PENNING IONIZATION STUDIES USING
A CROSSED-BEAM TECHNIQUE

by

John Stephen Howard

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ABSTRACT
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A modulated crossed-beam apparatus for the investigation of Penning ionization at thermal energies has been designed and constructed. Details are given for the production of a beam of helium metastable atoms by electron impact excitation. The production of well-collimated neutral beams of stable species using multichannel capillary arrays is analyzed, and preliminary measurements on the performance of one such array are presented. Production of atomic hydrogen by thermal dissociation of $H_2$ is discussed.

A detection system is described which collects product ions and separates those due to ionization of beam particles from those due to ionization of residual gas. Preliminary analysis of the appropriate operating conditions for the pulse counting system is presented.

To determine the types and abundances of ions produced in He*-neutral collisions, a magnetic sector mass
spectrometer has been designed. Extraction of the product ions from the interaction region and subsequent acceleration and steering of these ions through the spectrometer are analyzed.
Table of Contents

I. Introduction 1
II. The Crossed-Beam Apparatus 4
   A. Preliminary Design Considerations 4
   B. Vacuum System 8
   C. Internal Apparatus 11
III. Target Beam Formation 15
   A. Stable Species 15
      1. Gas Inlet System 15
      2. Principles of Beam Formation by Long Tubes 15
      3. Bendix Glass Array Properties 20
      4. Preliminary Measurements with the Glass Array 21
   B. Unstable Species 23
      1. Atomic Hydrogen 24
      2. Atomic Oxygen 27
IV. Total Ion Collection 28
   A. Apparatus 28
      1. Total Ion Collector (TIC) 28
      2. Calibration Electron Gun 29
      3. Counting System 30
   B. Operating Procedure 33
      1. He*-Neutral Collisions 33
      2. Electron-Neutral Collisions 34
   C. Preliminary Measurements 38
V. Mass Spectrometer Studies 46
   A. Need for a Mass Spectrometer 46
   B. Selection of the Type of Mass Spectrometer 47
CHAPTER I: Introduction

When a metastable particle $R^*$ collides with a neutral particle $AB$ whose ionization potential is less than the excitation energy of $R^*$, energy transfer may occur leading to one of the following chemiionization reactions:

\[
\begin{align*}
R^* + AB &\rightarrow RAB^+ + e^- \\
RA^+ + B + e^- &\quad (b) \\
R + AB^+ + e^- &\quad (c) \\
R + A^+ + B + e^- &\quad (d)
\end{align*}
\]

Reactions (c) and (d), in which metastable particle $R^*$ is de-excited to the ground state, are known as Penning ionization.

Experimental studies of Penning ionization are important for several reasons:

1. Penning ionization occurs in planetary atmospheres (Ferguson and Schluter, 1962; McElroy, 1965; Patterson, 1967). Successful explanation of the physical processes occurring in these atmospheres requires information from laboratory studies of Penning reactions.

2. Penning ionization is often present in laboratory environments, such as flowing afterglows (Fehsenfeld et al., 1965), and must therefore be considered in order to gain a more complete understanding of these environments.

3. Information from these experiments is helpful in evaluating theoretical descriptions of Penning ionization (Ferguson, 1962; Bell 1970; Bell et al., 1968; Fujii et al., 1970; Miller, 1970; Matsuzawa and Katsuura, 1970).
Both afterglow techniques and beam techniques have been used in laboratory investigations of Penning ionization. Afterglow methods may be subdivided into two types: the static, or time-dependent, afterglow (Benton et al., 1962) and the flowing, or spatially-dependent, afterglow (Schmeltekopf and Fehsenfeld, 1970; Bolden et al., 1970). Static afterglow techniques involve the excitation of a gas containing a small concentration of some reactant species. When the source of excitation is removed the system relaxes back to equilibrium. The period of time between the removal of the excitation mechanism and equilibrium is known as the afterglow, and it is during this period that Penning ionization analysis can most easily be performed. The static afterglow method suffers from the disadvantage that both the gas and the impurity species are exposed to the excitation mechanism. Consequently the reactant may be excited or ionized (or dissociated, if molecular) in unknown amounts.

Flowing afterglow systems do not subject the reactant species to the active discharge. A gas is forced to flow down a long tube in which a discharge is struck. Downstream from the discharge a reactant is injected, and any changes in concentration among the species can be monitored using optical techniques or mass spectrometer analysis.

Beam techniques involve the passage of a collimated beam of metastable particles through neutral target particles. These target particles are either confined within a chamber (Sholette and Muschlitz, 1962; Dunning and Smith, 1970) or are themselves formed into a beam which intersects the metastables at right angles (Hotop and Niehaus, 1968).
Unlike the afterglow systems, beam techniques permit investigation of the angular distribution of scattered metastables and the angular and energy distributions of Penning electrons. Furthermore, the dependence of collision properties upon the relative velocity between reactants can be studied. The crossed-beam technique also possesses a distinct advantage over the beam-gas cell technique, since chemically unstable target species can be studied.

As a consequence of the advantages that a crossed-beam technique possesses over the afterglow and beam-gas cell techniques, it was decided to construct a high vacuum crossed-beam apparatus, which is described in the next chapter, for the purpose of investigating the properties of chemiionization, with special emphasis on Penning reactions.
CHAPTER II: The Crossed-Beam Apparatus

In this chapter preliminary considerations which influenced the overall design of the crossed-beam apparatus are first discussed. A detailed description of the apparatus then follows which includes the vacuum system and the internal equipment required to conduct experiments on Penning ionization.

(A) Preliminary Design Considerations

It was decided to investigate collisions between thermal energy neutral particles which are present in planetary atmospheres. Although a number of metastables will ultimately be investigated, helium metastables were chosen as the species with which the initial experiments will be conducted. Several targets will be employed, including molecular nitrogen, hydrogen, and oxygen and certain chemically unstable species such as atomic hydrogen and oxygen.

The initial experiments will attempt to determine (1) total absolute Penning ionization cross sections involving a helium metastable beam containing a mixture of $2^3S$ and $2^1S$ levels and long-lived Rydberg levels with large principal quantum numbers, and (2) absolute cross sections for helium metastable beams composed of one particular excited level. Although several such cross section measurements have previously been made using the techniques described in Chapter I, there is justification for repeating a number of them since conflicting results have been obtained. In particular the flowing afterglow experiment of Schmeltekopf and
Fehsenfeld (1970) gives different values for He(2\textsuperscript{1}S)-He(2\textsuperscript{3}S) cross section ratios than do the beam experiments of Sholette and Muschlitz (1962) and Dunning and Smith (1970).

The measurements of Penning ionization cross sections will be based upon the fact that the number of reactive collisions per second \( S \) equals the difference between the original incident metastable intensity \( I_\star \) and the attenuated metastable intensity \( I \) after passage through the neutral beam:

\[ S = I_\star - I \]  

However, \( I \) and \( I_\star \) are also related by

\[ I = I_\star e^{-n_T \sigma \lambda} \]  

where \( n_T \) is the number density of targets, \( \lambda \) is the effective path length of metastables through the neutral targets, and \( \sigma \) represents the total cross section for reactions which attenuate the metastable beam. Since in general a cross section varies with particle energies (or velocities) the \( \sigma \) of equation (2) is actually an apparent cross section representative of the distribution of velocities in the beams.

If the product \( n_T \sigma \lambda \) is much less than unity, the exponential of equation (2) may be expanded to give

\[ I = I_\star (1-n_T \sigma \lambda) \]

so that equation (1) becomes

\[ S = n_T \sigma \lambda I_\star \]  

Equation (3) was derived assuming that \( S \) represented the
metastable beam attenuation. However, if product ions resulting from He*-neutral collisions are measured, S represents the product ion count rate and $\sigma$ represents the cross section for ionization. In addition, if Penning ionization is the dominant mechanism by which ions are produced then $\sigma$ represents the cross section for Penning ionization.

The value of $\lambda$ is not simply the geometrical path length $\lambda'$ of metastable atoms through the neutral beam because the target beam atoms are in motion. If metastables and target particles approach each other with average relative velocity $\bar{v}$, the effective path length can be expressed as

$$\lambda = v_r (\lambda'/\bar{v}_m)$$

where $\lambda'/\bar{v}_m$ is the time required for a metastable atom travelling with velocity $\bar{v}_m$ to traverse the neutral beam.

An estimate for $S$, the Penning ion count rate, will be based upon the following assumptions:

1. He*-H collisions are considered.
2. The interaction path length is taken as $\lambda = \lambda' = .5$ cm.
3. The ionization cross section $\sigma$ is assumed to be $22 \times 10^{-16}$ cm$^2$, which is a typical value for Penning ionization cross sections (Shaw et al., 1971).
4. The number density $n_H$ for an H-atom beam which is produced by a high temperature oven is about $10^9$/cm$^3$ (Fite and Brackmann, 1958).
(5) Ground state He atoms, produced by a multichannel array similar to those discussed in Chapter III, are excited by electron impact in the manner shown in Figure (1). It is expected that about $10^8$ metastables per second will be produced if the multichannel array produces a beam density of $10^{10}/\text{cm}^3$ along the beam axis.

Using these assumptions in equation (3) gives

$$S = 110 \text{ ions/second}.$$ 

This expected signal may be compared with the number of ions per second $S_b$ resulting from He*-background gas collisions. For a background density of $n_b$,

$$S_b = n_b \sigma \lambda_b I_*.$$  \hspace{1cm} (5)

The path length over which background ions will be collected is $\lambda_b = 3.75 \text{ cm}$, which corresponds to the diameter of the ion detector situated over the interaction region. If $\sigma = 22 \times 10^{-16} \text{ cm}^2$,

$$S_b = 8.2 \times 10^{-7} n_b \text{ background ions/sec}.$$ 

If the total multichannel array throughputs, which are on the order of $10^{17}$ particles/second (see Chapter III), are allowed to contribute to the background gas density then $n_b$ will be on the order of $10^{11}/\text{cm}^3$, even if a 600 liter/sec diffusion pump assembly is used to help evacuate the collision chamber. This density leads to

$$S_b = 8.2 \times 10^4 \text{ background ions/sec}.$$
The background count rate is much greater than the count rate expected from Penning ionization reactions.

These considerations led to the requirement that the crossed-beam apparatus should provide a small background gas pressure of about $5 \times 10^{-9}$ torr in the vicinity of the interaction region. Such a pressure would greatly reduce the background ion count rate and enable the data handling system described in Chapter IV to be used with relative ease.

(B) Vacuum System

In view of the large gas throughputs of the beam sources it was decided to construct a differentially pumped vacuum system, shown in Figures (1) and (2). The six rectangular apertures separate one differential pumping region from another and provide beam collimation. Most of the background gas particles emitted by the neutral beam sources are pumped out of the system through vacuum pumps located under chambers C1 and C2. The second and third differential pumping regions located along each beam path successively reduce the background gas pressure until $5 \times 10^{-9}$ torr is achieved in the region where the two beams cross.

The rotary pumps evacuate the system to a pressure of about .02 torr. The ball valve (see Figure 2) will normally be open enabling these pumps to operate in parallel on both manifold sections. However, if the beam source chambers are operated at high pressures, the manifold pressure may rise enough to cause a substantial increase in the interaction region pressure. In this case the ball valve will be closed,
Figure 1
The Crossed-Beam Apparatus

Titanium getter pump chamber

60° sector magnet

quadrupole lens pair
einzell lens
interaction region
faraday cup

scattering chamber

target beam chamber

source chamber

pivot point
multichannel array
tungsten filament
solenoid
calibration tube
depletion electron
gun
detector
slice
collision chamber
quench chamber
gas phase electrodes
array holder
helium source chamber
accelerating electrodes
internal partition
mechanical chopper wheel
C1 C2 C3 C4 C5 C6
To chamber: → C1 → C2 → C3 → C4 → C5 → C6

- Pump stack for N₂ (liter/sec)
- Liquid trap N₂
- Chevron valve
- Diffusion pump
- Manual valve

Leak check valve → Air vent valve → Zeolite trap → Cylindrical stainless steel manifold → Autopneumatic valve → Rotary pump (18 cfm)

Thermocouple gauge → Ball valve → Thermocouple gauge → Leak check valve

Figure 2
Figure 3

Distilled and city water systems for diffusion pumps.
thus forming two independent manifold sections. The larger rotary pump (18 cfm) will then evacuate only that part of the manifold leading to the higher pressure chambers C1, C2, C3, and C4, while the smaller pump (5 cfm) acts separately on C5 and C6. In this manner C5 and C6 are not subjected to a high manifold pressure.

Six oil diffusion pumps then reduce the pressure to $5 \times 10^{-9}$ torr in the interaction region. All diffusion pumps are water-cooled using a recirculating distilled water system (Figure 3). A chevron type baffle is situated directly above each diffusion pump to help prevent diffusion pump oil from reaching the vacuum chambers. In addition a liquid nitrogen-cooled trap hangs under each chamber directly above the baffle. Any oil vapor that has succeeded in getting past the baffle will condense on the trap.

To provide additional pumping at the collision chamber a getter pump was constructed and placed as shown in Figure (1). The portion of the target beam which does not undergo a reactive collision with the helium beam can enter the getter pump and, if the beam is not an inert gas, can be "pumped" by the usual gettering action of a titanium-coated surface. In the event that an inert gas target beam leads to a high collision chamber pressure, an oil diffusion pump can be placed underneath the getter pump chamber to help reduce this pressure.

Two additional measures were taken to attain high vacuum. All vacuum seals on the chambers were made with 1/16" diameter indium wire which, when flattened between two stainless steel flanges, cold welds to the two pieces
of metal. Because high purity indium (99.99%) outgases very little, pressures to $10^{-10}$ torr are attainable. Also, all vacuum chambers, constructed of stainless steel, were electro-polished. This procedure removed dirty surface layers and exposed the clean underlying surface.

The vacuum system is protected by an automatic safety system which includes the following features:

1. Zeolite traps are situated between the rotary pumps and vacuum manifold to collect any oil that may back-stream toward the vacuum chambers.

2. If the liquid nitrogen in one of the traps falls below a preset level the trap is automatically filled from a 160 liter dewar of liquid nitrogen.

3. If the 160 liter dewar becomes empty a second dewar is activated. If both dewars become empty the diffusion pumps will shut off.

4. If the distilled water to the diffusion pumps falls below a preset flow rate the diffusion pumps and water pump will shut off and the diffusion pumps will be quick-cooled with the city water system (see Figure 3).

5. If an electric power failure occurs for longer than five seconds the entire system shuts down and the diffusion pumps will be quick-cooled with city water. Two autopneumatic safety valves, located between backing pumps and zeolite traps, will automatically close to prevent the system from venting to atmospheric pressure through the backing pumps.

6. If a large leak develops in the vacuum system so that the manifold pressure rises above a preset level all
portions of the system will shut down except the distilled water flow.

(7) If either backing pump fails the autopneumatic valve closes and, if manifold pressure rises above the preset level, the entire system shuts down (except distilled water flow).

(C) Internal Apparatus

The helium beam is formed by flowing helium gas through a Bendix multichannel glass array. The array is composed of \( 4 \times 10^6 \) glass capillaries, each one being .025" in length and 2 microns in diameter. These capillaries are parallel with each other and with the desired beam axis and are evenly distributed within a 5mm x 5mm cross-sectional area. For a given total flow rate such a source produces better collimation along the desired beam axis than a single aperture (See Chapter III).

Enroute to the interaction region the helium atoms pass through the middle of a spiral-shaped tungsten filament (Figure 1). Electrons emerging from the heated filament are confined by a solenoidal magnetic field to travel collinearly with the helium beam. All electrons are accelerated to the desired energy (50-80 ev) by applying an electrostatic field between electrodes A1 and A2, shown in Figure 1. The large relative velocity between the fast-moving electrons and the helium atoms results in many collisions, some of which produce excitation of helium atoms. Most of the excited particles quickly decay
back to the ground state, typically in times less than $10^{-8}$ seconds, but those atoms excited to the $2^3S$ and $2^1S$ metastable states and those with large principal quantum numbers have lifetimes sufficiently long to enable them to arrive at the interaction region before decaying. However, Hotop and Niehaus (1968) have pointed out that direct excitation of high-lying Rydberg levels from the ground state is not very probable and such states may therefore be neglected in ionization studies.

The helium beam, now composed of atoms in the $1^1S$, $2^3S$, and $2^1S$ states, flows along the axis of a closed glass spiral which surrounds the beam path as in Figure (1). The spiral, made from Pyrex glass tubing, contains helium gas within which a discharge is struck. Helium radiation passes out through the walls of the tubing and into the helium beam. This radiation may be absorbed by the metastables, exciting them to higher states. The $2^1S$ atoms which have been excited decay preferentially to the ground state by electric dipole radiation so that in effect they have been "quenched", i.e. removed from the beam. If sufficient radiation is supplied by the helium discharge then all of the $2^1S$ atoms may be quenched. The $2^3S$ atoms may also be excited to higher levels but subsequent decay returns them to the $2^3S$ level, which is the ground state for the triplet system of helium.

A stable species target beam, also formed by multichannel arrays, flows toward the helium beam. In transit to the interaction region the target beam is modulated by a rotating toothed chopper wheel which helps separate
signal ions from background ions (See Chapter IV). Formation of neutral beams composed of chemically unstable atoms will be discussed in the next chapter.

The helium beam and the modulated target beam intersect at right angles. An electric field applied across the interaction region extracts product ions into either a particle multiplier for total ion measurement (Chapter IV) or into a mass spectrometer for mass analysis (Chapter V).

The metastable atom intensity is measured by placing an atomically clean tungsten surface in the path of the metastables and measuring the rate at which secondary electrons are ejected from the surface. Ground state atoms will not cause electrons to be ejected since they do not possess enough energy to overcome the work function of the metal surface, which is typically 5 eV. If the ejection efficiencies for He$^1 \text{S}$ and He$^3 \text{S}$ atoms, denoted by $\gamma_1$ and $\gamma_3$ respectively, are known then the singlet and triplet contributions to the total metastable beam can be found. The triplet contribution $I_3$ can be found by quenching all singlets with the helium discharge lamp:

$$I_3 = \frac{I'_3}{\gamma_3}$$

(6)

where $I'_3$ is the measured current due to secondary electron ejection. If the helium discharge is turned off then the measured current $I'$ is due to both singlets and triplets, so that

$$I' = \gamma_1 I_1 + \gamma_3 I_3.$$

(7)
Using equation (6) in equation (7),

\[ I_1 = (I' - I'_3)/\gamma_1 \]
(A) Stable Species

(1) Gas Inlet System

Since stable gases can be stored in high-pressure tanks, the gas inlet system for such species is relatively easy to construct. Figure (4) shows the essential features. With the needle valve closed, the manifold is evacuated to about .02 torr using the rotary pump. Valve RP is then closed and valve FV is opened so that the desired target gas can enter the manifold and fill tank No. 1 to the required pressure (typically 50 to 500 torr) through valve T1. By repeating this procedure tank No. 2 can be filled with a different gas, thus permitting a rapid change from one target gas to another. After the appropriate choice of target gas has been made, the needle valve is opened and gas flows through flexible stainless steel tubing to a moveable multichannel glass array mount. The mount permits the beam to be directed accurately toward the interaction region in both the vertical and horizontal directions by rotation about a pivot point located in the center of the array (Figure 4).

(2) Principles of Beam Formation by Long Tubes

Several devices have been used to form molecular beams, the three most widely used being the effusion source, the nozzle source and the multichannel source. Figure (5) illustrates these devices.
Figure 4
Gas inlet system
Figure 5
Neutral beam sources.
The effusion source is essentially a small aperture located in the wall of a gas-filled container, or "oven". Molecular flow through the aperture occurs when the mean free path \( \lambda \) of the gas exceeds the aperture dimensions. The intensity distribution as a function of angle \( \theta \), shown in Figure (5), is governed by the equation

\[
I(\theta) = n\bar{v}A \cos \theta / 4\pi r^2 \text{ particles/cm}^2 \text{-sec}
\]

where \( n \) is the number density of gas molecules in the oven, \( \bar{v} \) is their average velocity, \( A \) is the aperture area, and \( r \) is the distance from aperture to observer. A major weakness of this arrangement is the fact that the angular width of the beam is large, so that only a small fraction of the effusing gas is utilized in a collimated beam.

The nozzle source operates at higher pressures producing viscous flow instead of molecular flow. In passing through the converging-diverging nozzle, random velocities of the gas molecules are effectively converted into directed flow at supersonic velocities. As a result the angular width of the beam is smaller with more particles directed near \( \theta=0 \). Axial intensity gains of one hundred over effusion sources are common. However, the nozzle source is much more difficult to construct and operate than effusion or multichannel sources. In addition the velocity distribution in the beam, which is shifted toward higher velocities and is greatly reduced in width, cannot easily be predicted but must be experimentally determined.
The multichannel source consists of a parallel array of tubes packed closely together and having small diameter-to-length ratios. A large number of atoms which exit from these tubes have velocity vectors near $\theta = 0$ so that axial intensity gains of ten or more over effusion sources are easily obtainable. Although such gains are somewhat lower than for nozzle sources, multichannel arrays are easier to operate and produce a well-known velocity distribution. Several groups have investigated the characteristics of beams emerging from multichannel arrays, notably Giordmaine and Wang (1960), Hanes (1960), Johnson et al. (1966), and Zugenmaier (1965).

Giordmaine and Wang developed a theory which predicted the centerline intensity $I_t(0)$ and the beam half-width at half-maximum intensity $\theta_{1/2}$ for cylindrical tubes. They considered two limiting cases: (a) a transparent source (tube length $L \ll \lambda$) and (b) opaque source ($L \gg \lambda$). The transparent source assumes that particle-wall and particle-particle collisions in the tube play a negligible role, thereby resulting in an effusive situation with centerline intensity

$$I_t(0) = n\bar{v}a^2/4r^2 \text{ particles/cm}^2\text{-sec} \quad (8)$$

and beam half-width

$$\theta_{1/2} \approx 1.68 \ a/L$$

where $a$ is the tube radius. The opaque source takes into account both particle-wall and particle-particle collisions within the tube. The resulting formulas for centerline
Intensity and beam half-width are

$$I_t(0) = \frac{(3\pi a N/\eta)^{1/2}}{8 \cdot \sqrt{2} \cdot \delta} \text{ particles/sr-sec}$$

$$= \frac{(3\pi a N/\eta)^{1/2}}{8 \cdot \sqrt{2} \cdot \delta r^2} \text{ particles/cm}^2\text{-sec} \quad (9)$$

and

$$\theta_s = \left( \frac{3N/a\overline{v}}{\delta^2} \right)^{1/2} 2^{3/4} \frac{\delta}{1.78} \quad (10)$$

where \( N \) is the number of molecules flowing through the tube per second and \( \delta \) is the molecular diameter. Typically \( a \) is a few microns and \( L \) is ten to \( 10^4 \) times larger. However, Hanes (1960) pointed out that the requirement of \( L \gg \lambda \) is too severe. He maintained that in the collimating tubes a density drop occurs until, at some distance \( L' \) from the exit, \( L' \) becomes about equal to \( \lambda \). This remaining portion of the tube, \( L' \) in length, acts as the collimator while the initial portion of the tube is simply a flow resistance. Both Giordmaine and Wang and Hanes assumed that the gas density at tube exit was zero. Zugenmaier (1965) included a more realistic situation of a non-zero exit density and found that although \( I_t(0) \) as given in equation (9) was still valid \( \theta_s \) of equation (10) was too small by a factor of two, so that the proper expression for the half-width should be

$$\theta_s = \left( \frac{3N/a\overline{v}}{\delta^2} \right)^{1/2} 2^{7/4} \frac{\delta}{1.78} \quad (11)$$

In addition, Zugenmaier found the total integrated intensity over all \( \theta \) to be twice as large as Giordmaine and Wang had
If M tubes are constructed parallel to each other and occupy a gross area A, with a ratio of total tube cross-sectional area to gross area of $\varepsilon$, then the total array intensity $I(0)$ can be expressed as

$$I(0) = M I_t(0)$$

$$= \frac{(3vaMQ/\pi)^{\frac{1}{3}}}{8^{4/2} \delta r^2}$$

where $Q = MN$ is the total flow, in molecules per second, through the array. In terms of the transparency $\varepsilon$,

$$I(0) = \frac{(3vQAe/\pi^2 a)^{\frac{1}{3}}}{8^{4/2} \delta r^2}$$

The beam width can also be expressed in terms of $Q$ and $\varepsilon$ as well:

$$\theta_{1/2} = 2^{7/4} 3^{\frac{3}{2}} \delta (N/\pi av)^{\frac{1}{2}}$$

But $N = Q/M = Q \pi a^2 / \varepsilon A$, so

$$\theta_{1/2} = 2^{7/4} 3^{\frac{3}{2}} \delta (aQ/\varepsilon vA)^{\frac{1}{2}}$$
(3) Bendix Glass Array Properties

The multichannel arrays used with the crossed-beam system were produced by the Bendix Corporation with the following properties:

\[ a = 1 \times 10^{-4} \text{ cm} \]
\[ L = .025" = .063 \text{ cm} \]
\[ \varepsilon = .5 \]
\[ A = .5 \text{ cm} \times .5 \text{ cm} \]

From these values it is evident that there are approximately \( 4 \times 10^6 \) tubes, all having a diameter-to-length ratio of \( 3.2 \times 10^{-3} \).

In order to obtain a reasonable estimate of the total conductance of the glass array, the following experiment was performed. With the needle value of the gas inlet system (Figure 4) completely open in order to minimize constriction to the gas flow, the decrease in gas pressure behind the array was monitored as a function of time. Initial pressure was \( P_0 = 12 \text{ torr} \). Conservation of mass then requires that

\[ P(t) = P_0 e^{-Ct/V} \quad (15) \]

where \( P(t) \) is the pressure after time \( t \), \( C \) is the conductance of the glass array and its connecting tubing, and \( V = 2.44 \text{ liters} \) is the total volume of the gas. After 68 minutes the pressure had fallen to 2 torr. Therefore equation (15) gives

\[ C = 1.06 \times 10^{-3} \text{ liters/second} \].
Correcting for the tubing conductance of \(8 \times 10^{-3}\) liters/sec, the array conductance becomes

\[ C_a = 1.2 \times 10^{-3} \text{ liters/sec} \quad (16) \]

When experiments are being conducted with the multi-channel array it is useful to know the pressure immediately behind the array, i.e. the driving pressure \(P_a\). Since there is no vacuum gauge at this position, \(P_a\) must be calculated indirectly. To a good approximation it may be assumed that all molecules flowing through the glass array are removed from the source chamber by the 570 liter/sec diffusion pump below this chamber. If the source chamber pressure, measured with an ion gauge, is \(P_s\) then

\[ P_a C_a = 5.7 \times 10^2 P_s \]

or, using equation (16),

\[ P_a = 4.75 \times 10^5 P_s \]

(4) Preliminary Measurements with the Glass Array

Because the glass array could be rotated easily about a pivot point located in the center of the array, intensity distribution measurements were conducted in the vertical plane, as shown in Figure (6). The glass array was aimed at angle \(\theta\) with respect to the neutral beam axis, and the portion of the beam corresponding to \(I(\theta)\) passed through the three
collimating slits. In the collision chamber this portion of the neutral beam was crossed by a 1000 ev electron beam of known intensity (see Chapter IV for details of the electron gun) and small diameter (.05 to .1 cm). Ions produced by electron-neutral collisions were recorded by a counting system (see Chapter IV). The ion count rate served as a measure of the neutral beam intensity.

Figure (7) shows preliminary results of the vertical intensity distribution measurements. It is evident from this figure that the multichannel array behaved qualitatively as expected. The curve corresponding to higher throughput, and thus higher source pressure $P_s$, has a higher intensity for a given angle, which was predicted by equation (13). Although arbitrary units are used on the vertical scale, the relative magnitudes between the two curves are correct. At $\theta = 0$ the ratio of intensities for these curves is

$$\frac{I_1(0)}{I_2(0)} \approx 2$$

This value may be compared with the theoretical predictions of equation (13):

$$\frac{I_1(0)}{I_2(0)} = \left( \frac{Q_1}{Q_2} \right)^{\frac{3}{2}} = \left( \frac{P_{s1}}{P_{s2}} \right)^{\frac{1}{2}} \approx 2.4$$
Figure 6

Procedure for determining multichannel array intensity distributions.
Figure 7: Vertical intensity distribution

Counts/sec (relative units)

Curve 1 (closed circles)
\[ p_s = 1.35 \times 10^{-5} \text{torr} \]

Curve 2 (open circles)
\[ p_s = 2.3 \times 10^{-6} \text{torr} \]
Table 1

Comparison of theoretical estimates for beam half-widths with measured half-widths for two different source chamber pressures $P_s$. Curves 1 and 2 are shown in Figure 7.

<table>
<thead>
<tr>
<th>curve</th>
<th>$P_s$ (torr)</th>
<th>$\theta_{\text{theory}}^{1/2}$</th>
<th>$\theta_{\text{measured}}^{1/2}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>$1.35 \times 10^{-5}$</td>
<td>$.815^\circ$</td>
<td>$1.2^\circ$</td>
</tr>
<tr>
<td>2</td>
<td>$2.3 \times 10^{-6}$</td>
<td>$.336^\circ$</td>
<td>$.7^\circ$</td>
</tr>
</tbody>
</table>
where use has been made of the fact that the throughputs $Q_{1,2}$ are proportional to the source chamber pressures $P_{1,2}$.

Beam half-widths for the two curves of Figure (7) are given in Table (1). This table also indicates the theoretical estimates for $\theta_1$ according to equation (14). The measured array half-widths appear larger than the theoretical estimates. However, these theoretical values inherently assume that the multichannel array subtends a negligible solid angle at the point where half-width measurements are being conducted, i.e. at the interaction region. In the present experimental arrangement this is not the case, for the array subtends a total angle of $0.5^\circ$ in the vertical plane. It is therefore expected that the measured half-widths will be on the order of $0.25^\circ$ larger than $\theta_1$ (theory). After correcting for the finite size, measured half-widths still appear somewhat larger than expected. This would be the case if scattering processes were occurring. For example, the small densely packed tubes may lead to collisional interactions among the particles immediately after these particles leave the tubes. This self-scattering would broaden the beam profile. Also, scattering effects may be present just prior to the first collimating aperture if reflected particles near the aperture edges interact with the beam particles.

(B) Unstable Species

The two most common methods of producing chemically unstable neutral species at thermal energies involve dissociation in (1) an electrical discharge and (2) a high
temperature oven. Although an electrical discharge source can be cooled, thereby producing target particles with smaller velocities, and hence greater target beam densities than a high temperature oven can produce, there is the possibility that photons and excited states of the unstable species may be produced. Thermal dissociation in a hot oven, however, retains the unstable neutrals in the ground state. Moreover, thermal dissociation techniques can yield extremely high dissociation fractions with relative ease.

(1) Atomic Hydrogen

The unstable neutral target which will be investigated initially is atomic hydrogen. The most well-known method of thermally dissociating H_2 is the procedure of Fite and Brackmann (1958). They constructed a tubular furnace from rolled tungsten sheet. H_2 was fed into one end, while the other end was blocked. A small aperture was placed in the side of the tube from which gas could effuse. When the tungsten was heated to a temperature near 2800°K over 90% of the resulting beam was found to be atomic hydrogen.

Determination of the dissociation fraction D can be made using mass spectrometric analysis of ions produced by electron-target beam collisions. With the furnace operating at room temperature, so that the beam is composed of only H_2, the signal due to H_2^+ ions is measured:

\[
S = \sigma \int_{H_2} H_2^+ H_2 e \tag{18}
\]

where \( \sigma \) is the ionization cross section for production of H_2^+.
H\textsuperscript{+} in the e-H\textsubscript{2} collisions, \( \ell \) is the path length of electrons through the target gas, \( n_{H_2} \) is the number density of the target beam, and \( i_e \) is the number of electrons per second traversing this beam. Using the relation

\[
n_{H_2} = \frac{I_{H_2}}{\bar{v}_{H_2}}
\]

(19)

where \( I_{H_2} \) is the number of \( H_2/\text{cm}^2\text{-sec} \) travelling at velocity \( \bar{v}_{H_2} \), equation (18) can be written

\[
S_{H_2} = \frac{\sigma_{H_2} \ell i_e I_{H_2}^c}{\bar{v}_{H_2}^c}
\]

(20)

The superscripts indicate that this experiment is conducted with a cold (300\(^\circ\)K) furnace. Now, with the furnace hot (2800\(^\circ\)K), the same experiment is run on the mixed beam of \( H_2 \) and H. Again the mass spectrometer signal for \( H_2^+ \) is measured:

\[
S_{H_2}^{\text{hot}} = \frac{\sigma_{H_2} \ell i_e I_{H_2}^{\text{hot}}}{\bar{v}_{H_2}^{\text{hot}}}
\]

(21)

(The effect of vibrationally excited \( H_2 \) on \( \sigma_{H_2}^+ \) will have to be considered in those instances when significant population of vibrational levels occurs.) But the dissociation fraction is defined as

\[
D = 1 - \frac{I_{H_2}^{\text{hot}}}{I_{H_2}^c}
\]

(22)
Using equation (22) and \( \bar{v} \propto (kT)^{\frac{1}{2}} \)

\[
\frac{S^C}{S^+_{\text{hot}}} = \left( \frac{T^\text{hot}}{H_2^+} \right)^{\frac{1}{2}} \left( \frac{H_2}{T^C} \right) \frac{1}{1 - D}
\]

where it has been assumed that the \( H_2 \) is in thermal equilibrium with the furnace so that the beam can be represented by the furnace temperature \( T \). Solving for \( D \) gives

\[
D = 1 - \frac{S^\text{hot}}{S^C} \left( \frac{T^\text{hot}}{H_2^+} \right)^{\frac{1}{2}} \left( \frac{H_2}{T^C} \right)
\]

This last expression gives \( D \) if the ratio of molecular ion signals from the mass spectrometer are known, since it is not expected that mass spectrometer collection efficiencies for hot \( H_2^+ \) and cold \( H_2^+ \) will differ.

Although the above method of Fite and Brackmann gives high dissociation fractions the H-atom intensities are typically \( 10^9/\text{cm}^3 \) which are a factor of ten less than multichannel arrays can produce. It should be noted, however, that the construction of a multichannel oven made from tungsten has been attempted (C. B. Lucas, private communication). Preliminary results indicate that densities of \( 10^{11}/\text{cm}^3 \) have been produced with a multichannel oven.
(2) Atomic Oxygen

Tungsten ovens are not suitable for thermal dissociation of $O_2$, since tungsten oxidizes rapidly at high temperatures. However, significant dissociation fractions have been obtained using furnaces constructed from iridium. Lo et al. (1969) obtained dissociation fractions of 98% for furnace temperatures of $2300^\circ K$ and pressures of approximately $5 \times 10^{-4}$ torr. It remains to be seen whether large values for the dissociation fraction can be obtained in similar ovens containing the higher furnace pressures of $>1$ torr needed for crossed-beam experiments.
CHAPTER IV: Total Ion Collection

Ions resulting from the interaction between two crossed beams are measured with the collection system described in Section A of this chapter. Section B discusses the utilization of this system in determining Penning ionization cross sections and target beam intensities. The final section presents preliminary measurements which have been performed.

(A) Apparatus

(1) Total Ion Collector (TIC)

The total ion collector is shown schematically in Figure (8). Ions formed at the interaction region are accelerated toward a Johnston particle multiplier by means of an electric field \( E \) established between the bottom electrode and grid G1. Further acceleration is then achieved by the application of appropriate voltages to grids G2, G3, and G4. All grids are constructed of .0003" diameter tungsten wire equally spaced across 1.375" diameter circular holes which are located in stainless steel electrodes. The separation distance between adjacent wires is .0197", resulting in an optical transparency of 98.5%. The potential difference between G1 and G2 is kept small to minimize penetration of field \( E_{12} \) into the interaction region. Grid G4 is biased about 18 volts negative with respect to the first dynode of the multiplier to ensure that secondary electrons ejected from this dynode
Figure 8
Total ion collection system

calibration electron gun

raised position used when He beam is in operation

focusing and accelerating electrodes

steering electrodes

electron tube

target beam (into page)

electron gun

total ion collector

extraction axis

chamber wall

G4

G3

G2

E12

G1

bottom electrode

target beam (into page)

electron gun

total ion collector

external shield

particle multiplier

faraday cup

disk electrode

inner cylinder

outer cylinder
are directed toward the remaining dynodes.

An external cylindrical shield surrounding the TIC is maintained at an appropriate potential to minimize any field penetration into the TIC, which might affect ion collection.

The complete TIC assembly can be raised and lowered by a micrometer drive located outside the vacuum chamber. This movement enables either the TIC or the mass spectrometer extraction system (see Chapter V), which is suspended underneath the TIC bottom electrode, to be located at the interaction region.

(2) Calibration Electron Gun

The electron gun used in target beam intensity measurements is shown in Figure (8). Electrons are emitted from an indirectly heated cathode and are focused and accelerated toward the interaction region by the electrode structure shown in the figure. Small adjustments in the beam direction are made with the steering electrodes. Typical beam diameters of .05 to .10 cm may be obtained at the interaction region.

With the exception of the two final steering electrodes the electron gun may be raised and lowered by a micrometer drive located outside the vacuum chamber. When target beam intensity measurements are to be made, the electron gun is positioned so that the electron beam can pass through the target beam. When the He* beam is to be used, the electron gun is raised so that it does not constitute an obstruction to the metastables.
A cylindrical metal tube is positioned as shown in Figure (8). This tube is maintained at the same potential as the final accelerating electrode A1 of the electron gun, thus ensuring that the electron beam can travel from A1 to interaction region without experiencing a change in energy.

Electron beam intensities are measured with the stainless steel faraday cup shown in Figure (8). The outer cylinder is maintained at the same potential as the interaction region, while the inner cylinder is biased 12 volts negative with respect to the ground potential disk electrode situated in the path of the electron beam. All electrons strike the disk and the resulting current is measured with an electrometer. The potential difference between inner cylinder and disk electrode prevents escape of secondary electrons from the disk.

(3) Counting System

Although the crossed-beam vacuum system is differentially pumped, the typical operating pressures at the interaction region correspond to number densities of about $2 \times 10^8$ background particles/cm$^3$, which are in many instances comparable with target beam densities. Therefore a significant number of ions will be produced by collisions with the background gas. A counting system must be devised to separate these background ions from the signal ions produced from the crossed beams.

This counting system must also minimize the effects due to variations of background pressure with time, which
result from irregularities in pumping speed. Background pressure fluctuations typically occur on a time scale given by

\[ \gamma_f = \frac{\text{volume of collision chamber}}{\text{pumping speed}} \]

\[ \gamma_f = \frac{156 \text{ liters}}{570 \text{ liters/sec}} = 274 \text{ msec} \]

In addition to these pressure fluctuations, long-term drifts often result from warming of the liquid nitrogen traps as the liquid nitrogen supply is consumed, since time periods between trap fillings are about one hour. The effects of these time-dependent variations in background pressure may be mitigated by the use of ac counting techniques. The target beam is modulated at 100 Hz using a four-bladed rotating chopper wheel. Since the mark-space ratio of the toothed wheel is unity, the beam has a 50\% duty cycle, i.e. it is permitted to pass through the chopper wheel for half of each modulation period. The modulation period of .01 second is much less than the time constant for background pressure fluctuations so that the background pressure can be treated as a constant during each cycle.

The general procedure for determining the signal is as follows. While the target beam is on, the particle multiplier records ions formed from this beam and the background gas. However, when the target beam is off only background ions are measured. If the counts resulting from "signal plus background" ions associated with the
first half of each modulation period are stored in one scaler and those from the "background" ions associated with the second half of the modulation period are placed in a second scaler, the signal counts may be obtained as the difference between the two scaler readings.

Figure (9) shows a block diagram of the counting system electronics. Output waveforms for several of the components are displayed in Figure (10). The chopper wheel rotation is monitored by a light-photocell combination. Pulse generator PG1 is triggered by the amplified photocell output and provides a square wave output pulse of variable delay and width. The delay time is adjusted to equal the time taken by the neutral particles to travel to the interaction region from the chopper wheel. The pulse width of PG1 is adjusted to be the same as the photocell output width.

Scaler SCI is gated on whenever PG1 emits a pulse, and it remains on until the pulse from PG1 ends. In this manner SCI can accept counts only when the target beam is on and can therefore count both signal and background ions. Scaler SC2 can accept counts only when the target beam is off. Only background counts are monitored by SC2.

Even though the delay time of PG1 takes into account the finite travel time of the neutral beam from chopper wheel to interaction region, those particles which possess higher velocities arrive at the interaction region sooner than slower particles. Consequently the particle multiplier count rate builds continuously from zero to a maximum value instead of making a discontinuous jump. It
Figure 9: Counting System
Figure 10

Output waveforms for several counting system components.
is desirable to count ions only during the portion of each half-cycle in which the count rate is constant since this portion corresponds to constant target beam intensity and to constant effective path length of interaction.

To circumvent this difficulty the output pulse of pulse generator PG2, which is triggered on every half-cycle, is delayed sufficiently long so that the target beam intensity may reach its maximum value. The pulse from PG2 then triggers the preset scaler PSS, whose output pulse is adjusted to be on only when the target beam intensity is a constant.

The discriminator D1 is gated on by the output from PSS. During this time D1 accepts any amplified multiplier pulses which have heights exceeding the threshold setting of D1. An output pulse of standardized height and width is produced by D1 for each of these multiplier pulses. These standardized pulses are fed directly to the appropriate scaler.

A timing system, shown in the lower portion of Figure (9), counts the number of times that PG1 emits a pulse. After a pre-set number of these pulses has been registered, an inhibiting signal is delivered to the discriminator, thereby stopping all discriminator output. The number of recorded events in each scaler is then printed out on paper tape.

(B) Operating Procedure

(1) He*-Neutral Collisions

The determination of absolute Penning ionization
cross sections by measurement of product ions requires total collection of these ions. A strong extraction field can be applied across the interaction region between the bottom electrode and grid G1 of the TIC since the neutral beam trajectories are not affected by externally applied electric fields. A strong field helps minimize ion spreading transverse to the desired extraction axis. This feature is desirable because the product ions are less likely to encounter one of the grid plates as they are accelerated toward the particle multiplier, which would prevent total collection.

Although the most appropriate operating potentials for the gridded electrodes have not yet been determined experimentally, those of Figure (11) are reasonable estimates since they are consistent with the requirements of Section A and since they minimize electrostatic focusing in the vicinity of the grid wires which might affect total ion collection.

(2) Electron-Neutral Collisions

Electron-neutral collisions are used during dissociation fraction measurements associated with hot furnaces (see Chapter III) and during target beam intensity measurements. Since determination of dissociation fractions requires the use of a mass spectrometer, discussion of the appropriate operating procedure for these measurements is included in Chapter V.

When target beam intensity measurements are being conducted, a strong extraction field cannot be applied
(a) He*-neutral collisions

<table>
<thead>
<tr>
<th>First dynode</th>
<th>G4</th>
<th>G3</th>
<th>G2</th>
<th>G1</th>
</tr>
</thead>
<tbody>
<tr>
<td>-3000</td>
<td>-3018</td>
<td>-3000</td>
<td>-2500</td>
<td>-2000</td>
</tr>
</tbody>
</table>

Bottom electrode | \( E_c \) | 0 |
| Voltage |

(b) Electron-neutral collisions

<table>
<thead>
<tr>
<th>First dynode</th>
<th>G4</th>
<th>G3</th>
<th>G2</th>
<th>G1</th>
</tr>
</thead>
<tbody>
<tr>
<td>-3000</td>
<td>-3018</td>
<td>-2000</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Bottom electrode | \( E_c \) | -15 to 15 |
| Voltage |

Figure 11
Electrode potentials for the total ion collector.
across the interaction region since the electron beam would be deflected away from the target beam. A number of alternative operating procedures can be employed. One such alternative is to pulse the electron beam on and off at a high frequency and collect product ions with a strong extraction field after the electrons have passed through the interaction region but before the ions have undergone significant transverse spreading. The length of time that the extraction field can be applied is governed by the arrival of the next pulse of electrons.

A second alternative, one which is presently being used, is based upon the determination of the thermal ion contribution to the total signal. In those instances where the target beam is composed entirely of an atomic species, all product ions will possess thermal energies so that a weak extraction field of a few volts per centimeter is expected to result in total ion collection (see Figure 11).

When the target beam is a molecular species, however, two kinds of ions are produced: thermal ions and energetic ions of dissociation. As a typical example electron-N$_2$ collisions will be considered. These collisions may result in the following ionizing reactions:

\[
e + N_2 \rightarrow e + N_2^{+i} + (i) \ e^' \quad (a)
\]

\[
e + N^+ + N + e' \quad (b)
\]

where \( i \) is the number of times that \( N_2 \) has been ionized. Reaction (a) produces thermal energy ions, while reaction
(b) produces dissociated $N^+$ ions which may possess significant kinetic energies (McDaniel, 1964). Hereafter, all $N^+$ ions resulting from reaction (b) will be referred to as energetic ions.

The procedure for determining molecular target beam intensities is as follows. With grid Gl of the TIC fixed at ground potential, the bottom electrode potential is varied from about -15 volts to +15 volts in small voltage increments. At each voltage setting the product ion count rate is recorded, and a plot is made of signal versus bottom electrode voltage. The resulting curve is expected to be of the form shown in Figure (12). For large negative potentials, all thermal energy and energetic ions will experience a retarding field which will prevent them from reaching the multiplier. As the retarding field strength is reduced, an increasing fraction of energetic ions will have enough energy to overcome the retarding field effect and reach the multiplier. As $E_c$ changes from a retarding to an accelerating field, all thermal energy ions will be collected, resulting in the marked increase in slope of Figure (12). As the accelerating field is further increased, the slope resumes the value
Figure 12

Expected ion collection characteristics for electron-neutral collisions.
that it possessed for $V_b < 0$, since collection of energetic ions is again the controlling factor. The dashed curve of Figure (12) represents the expected curve shape assuming no thermal ion contribution. Therefore the difference in heights $H$ between the solid curve and the dashed curve for $V_b > 0$ corresponds to the total thermal energy contribution $S_{th}$ to the multiplier signal.

Knowledge of $S_{th}$ can be used to find the target beam density $n_T$. As in Chapter II, $S_{th}$ can be written

$$S_{th} = \sigma_{th} n_T i_e \lambda \text{ions/sec} \tag{24}$$

where $i_e$ is the number of electrons per second crossing the target beam, $\lambda$ is the effective path length of interaction, and $\sigma_{th}$ represents the total cross section for molecular ionization. Solving equation (24) for $n_T$,

$$n_T = \frac{S_{th}}{\sigma_{th} i_e \lambda} \tag{25}$$

However, $\sigma_{th}$ can be written in terms of the total cross section for ion production from e-$N_2$ collisions $\sigma_{tot}$ and the cross section for dissociative ionization $\sigma_d$ as

$$\sigma_{th} = \sigma_{tot} - \sigma_d$$
so that equation (25) becomes

\[ n_T = \frac{S_{th}}{(\bar{v}_{tot} - \bar{v}_d) i_e l} \]  

(26)

Therefore if \( \bar{v}_{tot} \) and \( \bar{v}_d \) are known from previous experiments (Kieffer and Dunn, 1966), the target beam density is calculable. The target beam intensity follows immediately from \( I_T = \frac{n_T}{\bar{v}} \).

(C) Preliminary Measurements

(1) The Johnston particle multiplier pulse shapes were examined using an oscilloscope. Each pulse contained, in addition to the expected large single peak, several smaller peaks, as shown in Figure (13). After this multiplier signal passed through the amplifier, the secondary peaks often possessed amplitudes greater than the discriminator threshold setting. These unwanted peaks were then counted as if they were produced by separate ions, giving count rates which were too high. This problem was eliminated by adjusting the discriminator output pulse so that its width was greater than the particle multiplier output width. It was finally decided to set the discriminator pulse width at 100 nanoseconds, which
Figure 13

Observed particle multiplier output waveform
was two or more times longer than the multiplier output width. Upon resumption of experiments, an attempt will be made to eliminate the secondary peaks.

The lengthening of the discriminator pulse widths introduced a 100 nanosecond dead time $t_d$ into the counting system. However, the true count rate is related to the measured count rate by

$$S_t = \frac{S_m}{1 - t_d S_m} \text{ ions/sec}$$

or

$$S_t = \frac{S_m}{1 - 10^{-7} S_m} \text{ ions/sec}$$

where $S_t$ and $S_m$ are the true and measured count rates, respectively. For typical measured count rates of $10^4$ ions/sec, an error of only .1% is introduced by this dead time, and in addition, the length of time required to accumulate sufficient counts is not substantially increased.

(2) When the TIC and counting system components were operated without any beams running, it was found that about 12 counts/min, due to cosmic rays and amplifier noise, were registered for any multiplier voltage up to -3000 volts on the first dynode.

(3) The advantage of counting ions only during that part of pulse generator PGL's output which corresponds to constant target intensity has already been discussed in Section A. To determine the correct placement of the counting window a plot of multiplier count rate versus
elapsed time into a given half-cycle was made, employing the method shown in Figure (14). The preset scaler pulse width was set at .05 msec. By varying the delay of PG2 this small counting width was swept across the output of PG1, and the multiplier counts were recorded for several time increments. The counts were generated by crossing the neutral beam with an electron beam produced by the calibration electron gun discussed previously in this chapter.

The time \( t_i \) required by the \( i \)th neutral to travel from chopper wheel to interaction region is

\[
\begin{align*}
  t_i &= \frac{L}{v_i} \\
\end{align*}
\]

where \( v_i \) is the particle velocity and \( L = 36 \text{ cm} \) is the travel distance. It is therefore evident that the multiplier count rate versus elapsed time plot also is a measure of the velocity distribution of the neutral beam particles.

The resulting measurements are presented in Figure (15). The abscissa represents elapsed time into PG1's pulse and the ordinate represents the ion count rate relative to the maximum signal \( I_M \) for the points shown. The solid curve is a theoretical curve based upon the assumption that a molecular beam velocity dependence of

\[
f(v)dv \propto v^3 \exp(-mv^2/2kT)
\]

existed for the nitrogen beam. This curve represents the
Figure 14

Procedure for determining the correct placement of the counting window.
Figure 15: Signal saturation curve
ratio of the number of particles $N(t)$ possessing sufficient velocities to have arrived at the interaction region by time $t$ to the total number of particles $N$ found by integrating the expression in equation (27) over all velocities:

$$\frac{N(t)}{N} = \frac{\int_{v=L/t}^{\phi} f(v) dv}{\int_{0}^{\phi} f(v) dv}$$

(28)

Good agreement between theory and experiment exists, thus suggesting that the velocity distribution in equation (27) was valid for the target beam.

The multiplier signal saturates after 1.5 msec has elapsed into the pulse of PGI. Although the signal fall time after the target beam encountered a chopper wheel blade was not measured, it is reasonable to assume that 1.5 msec is needed.

(4) Preliminary experiments for the determination of $n_T$ have been considered utilizing the procedure of Section B. Figure (16) shows the results for electron-$N_2$ collisions. Curve 1 shows a plot of background count rate versus the bottom electrode potential $V_b$, while curve 2 is a similar plot of signal ions. These curves have the predicted sharp increase in slope for $V_b \approx 0$, as well as two distinct regions corresponding to energetic ions, as predicted by Figure (12).
Figure 16b

Curt 2
Figure 17b

Curve 4

Counts (relative units)

Voltage of the bottom electrode

$V_b$ (volts)
(a) No field between Gl and bottom electrode

(b) Small field between Gl and bottom electrode

Figure 18
An effect not predicted beforehand is the maximum at $V_b = 0$. This maximum is very pronounced in curve 1 and is more than 12% higher than the value at $V_b \geq 4$ volts. Curve 2 also exhibits a slight maximum although it is only about 5% greater than the value at 4 volts.

Figure (17) shows a similar plot for different operating conditions. The peak is again very pronounced in the background curve 3 and has disappeared for the signal ion curve.

If the slight maximum in curve 2 is due to a different effect than the sharper peaks in curves 1 and 3, then apparently there is an effect which alters the background count rate without affecting signal ions at $V_b = 0$. The probable explanation of this effect is based upon small field penetration through the grid wires of grid G1 into the volume between G1 and the bottom electrode. Figure (18a) shows this field penetration in terms of equipotential lines. If background ion produced at point i is directed upwards, it encounters an electric field component directed inward. This field alters the trajectory so that the particle passes through G1 without encountering the grid plate. If, however, a small field $E_c$ is applied as in Figure (18b) the penetrating field is cancelled, and any ion produced at position i experiences no net inward force. Consequently the ion collides with the grid plate and is not collected by the multiplier. Those ions produced by electron-neutral beam collisions are located near the center of G1 and do not experience this effect. Further measurements are necessary to verify the foregoing explanation.
The dotted line in Figure (16b) is an extrapolation of the energetic ion contribution to $V_b > 0$. The thermal ion contribution $S_{\text{th}}$ to the total signal corresponds to the difference in height $H$, as shown. Approximately $4.2 \times 10^4$ thermal ions were collected in six seconds of counting time. Therefore

$$S_{\text{th}} = 7 \times 10^3 \text{ ions/sec.}$$

Using equation (26) for $n_T$ gives

$$n_T = 6.4 \times 10^9 \text{ particles/cm}^3$$

where $V_{\text{tot}} = 0.88 \times 10^{-16} \text{ cm}^2$ and $V_d = 1.75 \times 10^{-16} \text{ cm}^2$ have been used (Kieffer and Dunn, 1966). Using $\bar{v} = 5 \times 10^4 \text{ cm/sec}$ for a $300^\circ\text{K}$ beam of $N_2$ gives a target beam intensity of

$$I_T = n_T \bar{v} = 3.2 \times 10^{14} \text{ /cm}^2\text{-sec} \quad (29)$$

This value can be compared with the theoretical estimate for the centerline intensity $I(0)$ given by equation (13). Using the multichannel array parameters listed on page 17 and $S = 3.75 \times 10^{-8} \text{ cm}$ (Dushman, 1965),

$$I(0) = 4.0 \times 10^{46} Q^{1/2}.$$ 

$Q$ is the total number of molecules passing through the array per second. In terms of the source chamber pressure and pumping speed,
\[ Q = P_s \cdot (570 \text{ liter/sec}) \text{ torr-liters/sec} \quad (30) \]

\[ = 1.2 \times 10^{-2} \text{ torr-liters/sec} \]

\[ = 4.68 \times 10^{17} \text{ particles/sec} \]

where, for curve 2 in Figure (16), \( P_s = 2.1 \times 10^{-5} \) torr.

The centerline intensity then becomes

\[ I(0) = 2.75 \times 10^{15} \text{ /cm}^2\text{-sec.} \quad (31) \]

A comparison of equations (29) and (31) indicates that the theoretical prediction is too large by almost an order of magnitude. However, it should be pointed out that the theoretical prediction for \( Q \) was based upon the assumption that the source chamber pressure \( P_s \) was related to the array throughput \( Q \) by equation (30). This relation would not be valid if gas leakage occurred through the multichannel array holder (see Figure 1) into the source chamber. If this leakage occurred then the following expression would be valid:

\[ Q + Q_{\text{leak}} = P_s \cdot (570 \text{ liter/sec}) \]

or

\[ Q = P_s \cdot (570 \text{ liter/sec}) - Q_{\text{leak}} \quad (32) \]

A large \( Q_{\text{leak}} \) would result in a much smaller value for the actual array throughput \( Q \), and as a result the predicted centerline intensity \( I(0) \) would be smaller and therefore
closer to the measured intensity. Further investigations are needed in order to verify this explanation.
CHAPTER V: Mass Spectrometer Studies

This chapter is concerned with the extraction of product ions from the interaction region, their transport to the spectrometer, and their subsequent mass analysis.

(A) The Need for a Mass Spectrometer

In collisions between excited atoms and neutral targets, several ionization processes may occur. For instance, in a collision with an excited atom $R^*$, a molecular target $AB$ may undergo the reactions listed in Chapter I, producing ion types $RAB^+$, $RA^+$, $AB^+$, or $A^+$. If a mass spectrometer analysis is carried out on the ions resulting from $R^*-AB$ collisions, it is possible to tell which of the reactions is occurring and also how often one reaction occurs relative to the others, i.e. the branching ratios of various channels.

It was already mentioned in Chapter III that when an unstable atomic species is being used as a target, a mass spectrometer can be used to determine the dissociation fraction from the relation

$$D = 1 - \frac{S_{H_2^+}^{\text{hot}}}{S_{H_2^+}^{\text{cold}}} \left( \frac{T_{H_2}^{\text{hot}}}{T_{H_2}^{\text{cold}}} \right)^{1/2}$$

where the signals $S_{H_2^+}^{\text{cold}}$ and $S_{H_2^+}^{\text{hot}}$ represent mass analyzed $H_2^+$ signals at two given furnace temperatures. A mass spectrometer is therefore needed to measure the $H_2^+$ signals.
(B) Selection of the Type of Mass Spectrometer

Several kinds of mass spectrometers are in widespread use today, including magnetic sector analyzers, time-of-flight spectrometers, quadrupole and radio frequency spectrometers, multiple magnet systems, and other more exotic types. The most appropriate type of spectrometer for the crossed-beam apparatus must not only be able to achieve the goals of Section A but should do so in the simplest and most economical way.

The resolution requirements which must be met by the spectrometer are first considered. Resolution, or resolving power, is a measure of the ability of a spectrometer to distinguish between particles of different masses \( M \) and \( M + \Delta M \). Figure (19) illustrates the concept of resolution from a practical standpoint. Two peaks are shown, one corresponding to mass \( M \) and the other to mass \( M + \Delta M \). If the minimum between peaks \( h \) is less than \( 1/10 \) of the smallest peak height \( p \) then the two masses are said to be resolved.

The resolution \( R \) can be defined as

\[
R = \frac{M}{\Delta M} . \tag{33}
\]

For instance, if a spectrometer can successfully resolve mass 100 from mass 99, then

\[
R = \frac{100}{100-99} = 100 .
\]
Figure 19

Resolution of mass $M$ from mass $M + \Delta M$ is said to occur when $h \leq 1p$. 
If it can resolve mass 100 from 98, but not 99, then \( R_p = 50 \). If the target gases which are to be used in the Penning ionization experiments are examined with respect to the possible mass differences among product ions, \( R_p \) is found to be less than or equal to 10. Resolving \( \text{HeO}_2^+ \) from \( O_2^+ \), for example, would correspond to \( R_p = 9 \). This is a minimal requirement on any of the mass analyzers mentioned above.

The choice of mass analyzer can therefore be based upon ease of construction and simplicity of operation. Magnetic sector spectrometers easily meet these demands. A deflection angle of 60° is suitable for the crossed-beam apparatus. It should be pointed out, however, that any deflection angle within 30° of the one chosen would be acceptable.

(C) Selection of Operating Mode

Figure (20) shows a schematic of a 60° sector magnet. It is composed of two pole pieces separated by a gap width \( g \), through which the ion beam travels. Two opposing forces act on each ion inside the magnet, causing it to travel in circular orbits. The magnetic part of the Lorentz force, \( qvB \sin(v,B) \), is balanced by the centrifugal force, \( mv^2/r \), giving

\[ r = \frac{mv}{qB} \]  

(34)

where the ion of mass \( m \) is travelling at speed \( v \) in a mag-
Figure 20

Geometry of a sector magnet
netic field $B$. The ionic charge is $q$. From this equation it can be seen that the radius $r$ is proportional to the momentum $mv$ of the particle. Thus, the sector magnet alone is a momentum analyzer, not a mass analyzer. For instance, a particle of mass $m$ travelling at speed $v$ has the same momentum as a particle of mass $2m$ travelling at speed $v/2$, and these particles therefore travel on the same radius inside the magnet. To obtain the desired mass analysis, all particles of a particular mass must be given one distinct velocity. This can be done if all ions are accelerated to the same energy $E_b$. Then

$$E_b = \frac{mv^2}{2}$$

or

$$v = \left(\frac{2E_b}{m}\right)^{1/2}$$

giving, with the use of equation (34),

$$r = \left(\frac{2mE_b}{qB}\right)^{1/2}/qB .$$  \hspace{1cm} (35)

If the ions are accelerated by an electric field, the particles are given an energy $E_b = qV$, where $V$ is the accelerating potential. Equation (35) then becomes

$$r = \left(\frac{2mV}{qB^2}\right)^{1/2} .$$  \hspace{1cm} (36)

If it is assumed that all ions are singly charged, then each ionic mass travels on a radius that is proportional to $m^{1/2}$. 
The focusing properties of a sector magnet enable one specific mass to be detected. Figure (21a) shows three particles of mass \( m \) diverging from a point source and entering the magnetic field at different angles \( \alpha_i \). If the \( \alpha_i \) are close to 90°, then the masses will converge and focus at point D. The entrance and exit distances from the field boundaries are related by (McDowell, 1963)

\[
(1_{\text{en}} - r \cdot \text{ctn} \ 60^\circ)(1_{\text{ex}} - r \cdot \text{ctn} \ 60^\circ) = r^2 \cdot \csc^2 60^\circ \tag{37}
\]

or

\[
(1_{\text{en}} - \sqrt{3}r/3)(1_{\text{ex}} - \sqrt{3}r/3) = 4r^2/3.
\]

Choosing \( r = 15 \) cm for the magnet radius gives

\[
(1_{\text{en}} - 8.65)(1_{\text{ex}} - 8.65) = 300.
\]

Although equation (37) has been stated without proof, it will be verified for a particular case in Section F.

Two of the most common choices for \( 1_{\text{en}} \) and \( 1_{\text{ex}} \) are (Figure 21b,c)

\[
1_{\text{en}} = 1_{\text{ex}} = \sqrt{3}r = 25.98 \text{ cm (symmetric mode)}
\]

and

\[
1_{\text{en}} \to \infty, \ 1_{\text{ex}} = 8.65 \text{ cm (parallel beam mode)}.
\]

Either of these modes is compatible with the crossed-beam system, but the parallel beam mode seems more appropriate for two reasons. First, the product ions do not originate from a point source but from a relatively large interaction volume of 4mm x 5mm x 5mm, so that the parallel beam mode requires only that these ions be extracted and formed.
Figure 21

60° sector magnet focusing.
into a parallel beam. The symmetric mode, however, requires that the ions be extracted, focused to a point, and then allowed to diverge toward the spectrometer. The second advantage of the parallel beam mode is the fact that the magnet can be placed anywhere along the parallel beam path. Therefore $l_\text{en}$ can be chosen small, so that the ions traverse a much shorter distance from interaction region to spectrometer detector and thus have less chance of being scattered by background gas. Consequently the parallel beam mode seems more desirable, but because measurements using the mass spectrometer have not yet been conducted, the beam shaping and steering systems described in the next section were designed to be applicable to both modes.

(D) Formation of a Parallel Ion Beam

Figure (22) shows the apparatus to be used in the formation of a parallel ion beam. The extraction grids and the three-element electrostatic lens are attached to the bottom electrode of the TIC, as shown in the figure, while the quadrupole lens pair is attached to a side flange. When ion analysis is to be carried out, the micrometer drive raises the TIC above the interaction region and permits the extraction grids of the mass spectrometer system to be properly positioned. Since the product ions are to be given a significant energy before entering the mass spectrometer, the extraction region will necessarily be at a potential different from the spectrometer. The extraction region can be held at ground potential and the
Figure 22: Formation of a Parallel Beam
spectrometer floated at a large negative potential, or the extraction region can be maintained at a high positive potential and the spectrometer kept at ground. The second alternative was chosen since there is less danger to the experimenter if the high voltage is inside the vacuum system where it cannot accidently be touched. Also it is easier to isolate the extraction system from the collision chamber than to isolate the spectrometer chamber, which would in addition require a protective enclosure.

The operating voltage of the extraction region was chosen to be 1000 volts. This voltage is conveniently low, yet it is high enough so that any small initial variations in ion energies become negligible. If, for instance, one ion is produced with zero kinetic energy and another ion of the same mass has an energy of 10 ev, then the final energies for both ions, after acceleration, lie within 1% of each other.

The apparatus shown in Figure (22) was designed to have high transmission properties in an attempt to obtain total ion collection for each ionic mass.

(1) Extraction Region

The extraction region is composed of four highly transparent grids (98.5% optical) placed over 3 cm diameter circular apertures and made from .0003" diameter tungsten wires. When He*-neutral product ions are to be mass analyzed, a strong extracting field can be applied across the interaction region, thus preventing any significant spreading of product ions transverse to the desired ex-
traction axis. This procedure is directly analogous to the TIC extraction procedure. The specific operating potentials of grids S2 and S3 will be determined experimentally, but they are expected to be near 500 and 250 volts, respectively, since these voltages would minimize electrostatic lens action in the vicinity of the grid wires. Grid S4 will be at ground potential.

Different grid potentials will be used when measurements on the dissociation fraction of a mixed beam of molecular and atomic targets are made. Again, in analogy to the beam intensity measurements with the TIC, a weak extracting field of a few volts per centimeter will be used in order not to deflect the electron beam away from the target beam. Grids S2 and S3 will now be at about the same potential to prevent the strong accelerating field between S3 and S4 from penetrating to the interaction region. Although some of the more energetic ions of dissociation may not be successfully transmitted through the extraction region, signals due to these ions are not necessary for the determination of dissociation fractions. It is expected however that total transmission of thermal energy ions will occur.

(2) Three-element Lens

Even though the ion beam has been accelerated by a 1000 volt potential toward the mass spectrometer entrance, small transverse velocity components still exist for many ions. It is desirable to alter these diverging trajectories so that all ions are travelling directly toward the spectrometer entrance. The three-element lens shown in
Figure (22) can be used for this purpose. If the two outer electrodes are held at the same potential, the emerging ion beam retains the energy that it possessed prior to entering the lens. Such lenses are called unipotential, or einzel, lenses because only one voltage is needed for their operation. The middle electrode can be operated either above or below ground since focusing occurs in both cases according to the focal length formula (Paszkowsky, 1968)

\[
\frac{1}{f} = \frac{3}{16} \int_{z_o}^{z_i} \left( \frac{\varphi'(z)}{\varphi(z)} \right)^2 \, dz
\]

where \( f \) is the focal length, \( z_o \) and \( z_i \) are the object and image distances from the lens center, respectively, \( \varphi(z) \) is the potential at \( z \), and \( \varphi'(z) \) is the first derivative of the potential. Because the integrand is always positive, \( f \) is always greater than zero, which means that the lens is always converging, or focusing.

Since the cross-sectional area of the ion beam is to be kept as small as possible to more easily pass through the magnet gap, the middle electrode potential will be operated below ground. This makes the first portion of the lens focusing and the second portion defocusing, but since the focusing action has a larger effect each resulting trajectory is more convergent than the initial trajectory (see Figure 22), and each ion lies closer to the desired beam axis. If the middle potential was maintained above ground, the final ion displacement from the beam axis would be larger than the initial displacement, al-
though its trajectory would still be more convergent.

The most appropriate operating voltage which must be applied to the middle electrode to obtain a parallel beam will be experimentally determined by maximizing the detector signal for each mass.

(3) Quadrupole Lens Pair

The einzel lens is followed by a quadrupole lens pair which is primarily a beam shaping device with high transmission properties. Figure (22) shows the geometry of a quadrupole lens pair and typical beam trajectories in two perpendicular directions. It is evident from this figure that the focusing characteristics are astigmatic, i.e. the focal point in one plane will not coincide with the focal point in the other plane. In the horizontal (y-z) plane all ions first feel a converging force inside quadrupole lens QL1, then a drift space between the two quadrupoles, and finally a diverging force inside QL2. In the vertical (x-z) plane the ions feel a defocusing force, a drift space, and finally a focusing force. The diagonally opposing lens electrodes are usually run at identical potentials. However, in the event of minor beam misalignment with respect to the spectrometer, small differences in potential between opposing electrodes can be applied to correct the beam trajectory.

The effects of beam shaping may be predicted using matrix analysis of beam trajectories (see Appendix). For the following calculations the beam width at the entrance to QL1 is assumed to extend $\pm .7$ cm from the desired beam.
axis in both the vertical and horizontal directions. It is also assumed that the ions form a parallel beam which is properly aligned with the mass spectrometer. All electrode lengths are assumed to be 3 cm, and the distance between opposing electrodes is taken as 3.5 cm. The drift space length is 2 cm.

(a) Converging-Diverging Plane (y-z plane)

From equation (A9) of the Appendix, the off-axis distance \( y(z) \) and slope \( y'(z) \) at the exit from QL1 is related to the initial conditions \( y_o = \pm .7 \text{ cm and } y'_o = 0 \) by

\[
\begin{pmatrix}
  y \\
y' \\
Q1L
\end{pmatrix} =
\begin{pmatrix}
  \cos k_1 z & k_1^{-1} \sin k_1 z \\
-k_1 \sin k_1 z & \cos k_1 z
\end{pmatrix}
\begin{pmatrix}
y_o \\
y'_o
\end{pmatrix}
\]

where

\[
k_1 = a^{-1} \left( \frac{V_{ly}}{V_{ion}} \right)^{\frac{1}{2}}
\]

\( V_{ly} \) and \( a \) are defined in Figure (22), and \( V_{ion} \) is the potential corresponding to an ion beam of energy \( eV_{ion} \). Because of the relatively long electrodes and drift space, the electrode potentials are low, typically less than 75 volts from ground. The following potentials were found to be consistent with the desired effects on the ion beam:

\[
V_1 = \pm 50 \text{ volts}
\]

\[
V_2 = 62.5 \text{ volts}
\]
The upper sign corresponds to the y-z plane and the lower one to the x-z plane. These values give, for \( V_{ion} = 1000 \) volts,

\[
    k_1 = .128 \text{ cm}^{-1}
\]

\[
    k_2 = .143 \text{ cm}^{-1}
\]

The beam trajectory may now be calculated from equation (38):

\[
\begin{align*}
    \begin{pmatrix} y \\ y' \end{pmatrix} & = \begin{pmatrix} \cos (.384) & 7.81 \sin (.384) \\ -.128 \sin (.384) & \cos (.384) \end{pmatrix} \begin{pmatrix} \pm .7 \\ 0 \end{pmatrix} \\
    \begin{pmatrix} y' \end{pmatrix}_{QLL} & = \begin{pmatrix} \pm .65 \\ -.034 \end{pmatrix}
\end{align*}
\]

(39)

For the 2 cm drift space, according to equation (A2) of the Appendix,

\[
\begin{align*}
    \begin{pmatrix} y \\ y' \end{pmatrix} & = \begin{pmatrix} 1 & L \\ 0 & 1 \end{pmatrix} \begin{pmatrix} y_0 \\ y'_0 \end{pmatrix} \\
    \begin{pmatrix} y' \end{pmatrix}_{DRIFT} & = \begin{pmatrix} 1 & 2 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \pm .65 \\ -.034 \end{pmatrix} = \begin{pmatrix} \pm .582 \\ -.034 \end{pmatrix}
\end{align*}
\]

(40)
where the initial conditions for the drift space are the same as the exit conditions for QL1.

For QX2, using equation (A10) of the Appendix,

\[
\begin{pmatrix}
    y \\
    y'
\end{pmatrix}_{QL2} = 
\begin{pmatrix}
    \cosh k_2 z & k_2^{-1} \sinh k_2 z \\
    k_2 \sinh k_2 z & \cosh k_2 z
\end{pmatrix}
\begin{pmatrix}
    y_0 \\
    y'_0
\end{pmatrix}
\]

\[
= \begin{pmatrix}
    \cosh (.429) & 7.0 \sinh (.429) \\
    0.43 \sinh (.429) & \cosh (.429)
\end{pmatrix}
\begin{pmatrix}
    \pm.582 \\
    \mp.034
\end{pmatrix}
\]

or

\[
\begin{pmatrix}
    y \\
    y'
\end{pmatrix}_{QL4} = \begin{pmatrix}
    \pm.53 \\
    \mp.003
\end{pmatrix}
\]

(41)

Therefore, the exit conditions from QL2 are an off-axis displacement of \( \pm.53 \) cm with a slightly converging slope of \( \pm.003 \), which corresponds to an angle of \( 0^\circ 10' \), so it is evident that the ion beam can be considered a parallel beam in the y-z plane with a reduced transverse dimension of \( \pm.53 \) cm from the beam axis.

(b) Diverging-Converging Plane (x-z plane)

Calculations for this plane can be performed in the
same manner as for the y-z plane. Again, using $x_0 = \pm 0.7$ cm and $x'_0 = 0$,

$$
\begin{pmatrix}
  x \\
  x'
\end{pmatrix}
= 
\begin{pmatrix}
  \cosh(0.384) & 7.81 \sinh(0.384) \\
  0.128 \sinh(0.384) & \cosh(0.384)
\end{pmatrix}
\begin{pmatrix}
  \pm 0.7 \\
  0
\end{pmatrix}
= 
\begin{pmatrix}
  \pm 0.753 \\
  \pm 0.035
\end{pmatrix}
$$

$$
\begin{pmatrix}
  x \\
  x'
\end{pmatrix}
= 
\begin{pmatrix}
  1 & 2 \\
  0 & 1
\end{pmatrix}
\begin{pmatrix}
  \pm 0.753 \\
  \pm 0.035
\end{pmatrix}
= 
\begin{pmatrix}
  \pm 0.823 \\
  \pm 0.035
\end{pmatrix}
$$

$$
\begin{pmatrix}
  x \\
  x'
\end{pmatrix}
= 
\begin{pmatrix}
  \cos(0.429) & 7 \sin(0.429) \\
  0.143 \sin(0.429) & \cos(0.429)
\end{pmatrix}
\begin{pmatrix}
  \pm 0.823 \\
  \pm 0.035
\end{pmatrix}
= 
\begin{pmatrix}
  \pm 0.850 \\
  \pm 0.017
\end{pmatrix}
$$

In this plane a net off-axis displacement of $\pm 0.85$ cm results, with a converging exit slope of $\pm 0.017$, which corresponds to an angle of approximately $1^\circ$.

(E) Magnet Design and Operation

The proposed electromagnet to be used with the crossed-beam system is shown in Figure (23). Because the mass analyzed ions will be detected with a Johnston particle multiplier which is fixed in position, the magnetic field will be varied so that the different masses may each be successively focused into the detector. Since the magnet radius is 15 cm and the beam has experienced a 1000 volt accelerating potential, the required field as a function of $m/q$ is

$$
B_{gap} = (2mV/r^2)^{1/2} = 1.17 \times 10^{-5}(m/q)^{1/2} \text{ gauss}
$$
Figure 23
Electromagnet
where $B_{\text{gap}}$ is the field in the magnet gap. If the mass is expressed in atomic mass units and $n$ represents the number of times that the ion is ionized ($q = ne$) then

$$B_{\text{gap}} = 144 \left( \frac{MV}{n} \right)^{1/2} / r \text{ gauss}$$

$$= 303.6 \left( \frac{M}{n} \right)^{1/2} \text{ gauss} \quad (43)$$

Here $M$ is in amu. It can be seen that a magnetic field of 3000 gauss enables any mass $\leq 99$ to be focused into the detector, assuming $n=1$.

The pole piece area of Figure (23) is $A_p = 130 \text{ cm}^2$, as compared with a yoke cross section of $A_y = 62 \text{ cm}^2$. Therefore, the maximum field expected in the yoke is

$$B_y = A_y B_{\text{gap}} / A_p = 2.1 \times 10^3 \text{ gauss}$$

which is less than the saturation field for the yoke material (Armco ingot iron saturates at $2.16 \times 10^4$ gauss).

The gap width $g$ in Figure (23) should be larger than the vertical ion beam dimension if total ion collection is to be possible. Exit conditions from the second quadrupole lens were calculated in Section D. If these conditions are used as input for the drift space from QL2 to the magnet entrance, the vertical beam height entering the gap can be calculated.

$$\begin{pmatrix} x \\ x' \end{pmatrix} = \begin{pmatrix} 1 & 10 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \pm 0.85 \\ \mp 0.017 \end{pmatrix} = \begin{pmatrix} \pm 0.68 \\ \mp 0.017 \end{pmatrix} \quad (44)$$

where the drift space length was taken as 10 cm. The total vertical displacement is 1.36 cm.

If a total magnet gap width of 3.2 cm is chosen,
Figure 24

Magnetic field strength versus $u$.
(From Enge, 1967).
.635 cm of which corresponds to the spectrometer vacuum chamber wall thickness (see Figure 23), an opening of 2.56 cm is available for the ion beam.

The pole face dimension along the y-axis of Figure (23) was constructed so that the magnetic field through the ion beam would be constant. Enge (1969) has calculated the magnetic field variation as a function of perpendicular distance from the field boundary. Figure (24) shows his results. It is evident that if the ion beam remains more than one gap width from the magnet edges then it experiences a constant field to within 1%. The ion beam's horizontal dimension is 1.06 cm according to equation (41), and since the gap width is 3.2 cm, a minimum of 7.46 cm is required for the y-dimension of the pole face. This dimension was constructed to be 3" (7.62 cm).

The fringing field variation also exists in the region between QL2 and the magnet and between magnet and detector. Therefore, the ion beam will be deflected to some extent in these regions. This effect can be compensated for by adjusting the magnet position until maximum signal readings are recorded by the detector.

The magnetic field will be produced by current-carrying coil windings shown in Figure (23). A current of about 2 amps will be supplied to these 4000 windings which are made from #16 copper wire. In terms of the electromagnet parameters, the magnetic field in the gap is, using Ampere's law,

$$B_{\text{gap}} = \frac{10^4 NI}{(2.7*1^2 + 2.1_p + \mu_0^{-1})} \text{ gauss} \quad (45)$$

where

- \( N \) (number of turns) = 4000
- \( I \) (current) = 2 amp
\[ \mu (\text{Armco iron permeability}) = 4 \times 10^3 \mu, \text{at 20 gauss} \]
\[ \mu_s (\text{free space permeability}) = 4 \times 10^{-5} \text{ henry/meter} \]
\[ l_y (\text{length of yoke}) = 1.11 \text{ meter} \]
\[ l_p (\text{length of pole piece}) = 0.089 \text{ meter} \]
\[ g (\text{gap width}) = 0.032 \text{ meter} \]

These values give the desired maximum of 3000 gauss for \( B_{\text{gap}} \).

(F) Mass Selection and Detection

Although equation (37) was previously used to find the point at which focusing occurs for a mass selected ion, this focal point can easily be calculated by applying matrix techniques to a sector magnet. A derivation of the appropriate transfer matrix for particle trajectories through sector magnets can be found in the Appendix. The result is based upon the assumptions that (1) the entering beam has a small spatial extent compared to the bending radii in the magnet, (2) all particles enter nearly perpendicular to the field, and (3) any momentum spread in the beam is small. From equation (A23) of the Appendix

\[
\begin{pmatrix}
  y \\
  y' \\
  \Delta P/P
\end{pmatrix} =
\begin{pmatrix}
  \cos \alpha & r \sin \alpha & r(1-\cos \alpha) \\
  -r^{-1} \sin \alpha & \cos \alpha & \sin \alpha \\
  0 & 0 & 1
\end{pmatrix}
\begin{pmatrix}
  y_O \\
  y'_O \\
  \Delta P/P
\end{pmatrix}
\]

where \( \Delta P \) is the momentum spread, \( r \) is the bending radius, and \( \alpha \) is the sector angle. For a magnet with \( r = 15 \text{ cm} \) and \( \alpha = 60^\circ \), assuming that the entering beam is a parallel beam
of ±.5 cm horizontal extent,

\[
\begin{pmatrix}
  y \\
  y' \\
  \Delta P/P
\end{pmatrix}
= \begin{pmatrix}
  .5 & 7.5\sqrt{3} & 7.5 \\
  -\sqrt{3}/30 & .5 & .5\sqrt{3} \\
  0 & 0 & 1
\end{pmatrix}
\begin{pmatrix}
  \pm.5 \\
  0 \\
  \Delta P/P
\end{pmatrix}
\]

\[
= \begin{pmatrix}
  -\frac{1}{3} & 0 \\
  -\frac{\sqrt{3}}{2} & 0 \\
  0 & 0
\end{pmatrix}
\] if \( \Delta P/P \) is small \hspace{1cm} (46)

It was claimed in Section C that a drift space of 8.65 cm was needed after the magnet to bring all mass selected particles to a focus. To check this statement, the drift space transfer matrix is applied to the above results using an 8.65 cm drift space length:

\[
\begin{pmatrix}
  y \\
  y' \\
  \Delta P/P
\end{pmatrix}
= \begin{pmatrix}
  1 & 8.65 \\
  0 & 1
\end{pmatrix}
\begin{pmatrix}
  \pm.25 \\
  -\frac{\sqrt{3}}{260}
\end{pmatrix}
\approx \begin{pmatrix}
  0 \\
  -\frac{\sqrt{3}}{260}
\end{pmatrix}
\] (47)

The correct focal length is indeed 8.65 cm.

The actual size of the focal "point" can be calculated if assumptions (1) and (3) on page 62 are removed. If assumption (2) only is retained, the results of Part (c) of the Appendix can be used. Equation (A33) gives the relation for the image displacement \( W \) of a particle of radius \( r' \) in the magnet. \( W \) is measured with respect to the median ray trajectory as shown in Figure (A3).

\[
W = \left\{ x\left[ \sin\kappa + \cos\left(\kappa + \theta\right)\right] + r \cdot \cos\left(\kappa + \theta\right) - \cos\kappa \right\}\sin\kappa
\]
where
\[ \theta = \sin^{-1} \left( \frac{\Delta r + x_o \sin \alpha}{r} \right) \]
and
\[ x = (\Delta r + x_o) \cos \alpha + r \left[ 1 - \left( \frac{\Delta r + x_o}{r} \right)^2 \sin^2 \alpha \right]^{1/2} - r \]

Table (2a) shows the results of a calculation by R. Rundel (private communication) for the image width for various initial displacements of a specific mass from the beam axis, assuming that \( r = 15 \) cm. It is evident that if the detector slit of Figure (A3) has a width of \( \pm 0.006 \) cm from the median ray path and if it is placed at the median ray image position, then total ion collection of an ion beam with initial displacement \( \pm 0.5 \) cm should be possible. Table (2b) shows the image displacement of mass 52 (with radius \( r' = 15.3 \) cm) from mass 50 (with \( r = 15 \) cm), which corresponds to a resolution of \( M/\Delta M \approx 25 \). The displacements for mass 52 are typically \( 0.3 \) cm from mass 50. Therefore particles of mass 52 will not pass through a detector slit of width \( \pm 0.006 \) cm. The actual slit need not be as small as \( \pm 0.006 \) cm; it can, if desired, be \( \pm 0.05 \) cm to ensure total ion collection for a given mass.

The vertical height of the detector slit should be greater than the expected vertical height of the mass selected beam. A height of \( 1.0 \) cm allows ample clearance for the beam.
Table 2

Image displacement $W$ calculations using equation (A33).

2(a) Calculations by R. Rundel (private communication) for one specific mass deflected on 15 cm radius. A parallel beam mode is assumed.

2(b) Calculations for mass 52 relative to mass 50. Mass 50 is deflected on 15 cm radius. A parallel beam mode is assumed.

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<thead>
<tr>
<th>$x_0$ (cm)</th>
<th>$x_{final}$ (cm)</th>
<th>$\theta_{final}$ (°)</th>
<th>$W$ (cm)</th>
</tr>
</thead>
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<tr>
<td>0.25</td>
<td>0.123</td>
<td>0.827</td>
<td>-0.00157</td>
</tr>
<tr>
<td>-0.25</td>
<td>-0.127</td>
<td>0.827</td>
<td>-0.00156</td>
</tr>
<tr>
<td>0.5</td>
<td>0.244</td>
<td>1.654</td>
<td>-0.00598</td>
</tr>
<tr>
<td>1.0</td>
<td>0.475</td>
<td>3.31</td>
<td>-0.02502</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$x_0$ (cm)</th>
<th>$x_{final}$ (cm)</th>
<th>$\theta_{final}$ (°)</th>
<th>$W$ (cm)</th>
</tr>
</thead>
<tbody>
<tr>
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<td>0.45</td>
<td>1°</td>
<td>0.292</td>
</tr>
<tr>
<td>0.5</td>
<td>0.7</td>
<td>2° 35'</td>
<td>0.3</td>
</tr>
<tr>
<td>-0.5</td>
<td>0.2</td>
<td>-40'</td>
<td>0.32</td>
</tr>
</tbody>
</table>
(G) Collection Efficiency

In general the collection efficiency for a given type of ion will depend upon its mode of formation. As an example, consider the following case:

\[ R^* + T_2 \rightarrow R + T_2^+ + e \]
\[ R + T^+ + T + e \]
\[ RT_2^+ + e \]

If the measured mass spectrometer detector signals are denoted by primes and the actual ion production rates are unprimed, the following equations can be written:

\[
i' = \kappa \frac{i}{T_2^+} \]
\[
i' = \beta \frac{i}{T^+} \]
\[
i' = \gamma \frac{i}{RT_2^+} \]

where \( \kappa \), \( \beta \), and \( \gamma \) are the collection efficiencies associated with \( T_2^+ \), \( T^+ \), and \( RT_2^+ \), respectively. Also, the total ion current as measured by the TIC can be written as

\[
i_{TOT} = \frac{i}{T_2^+} + \frac{i}{T^+} + \frac{i}{RT_2^+} \]

or, using equations (48),
There are three unknowns (the collection efficiencies) and one equation. If the approximation is made that all thermal ions have equal collection efficiencies, then \( \alpha = \gamma \) and

\[
i_{\text{TOT}} = \alpha^{-1} i_{T_2^+} + \beta^{-1} i_{T_2^+} + \gamma^{-1} i_{R_T^2}
\]  

(49)

which reduces the unknowns to \( \alpha \) and \( \beta \).

Using the assumption that all thermal ions are collected with the same efficiency, \( \alpha \) may be determined separately by comparing the mass spectrometer and TIC signals in those circumstances when only thermal ions are produced. Using argon, for example, as the target gas leads to the following expression for:

\[
\alpha = i_A^+ / i_{A^+}
\]

(51)

where \( i_{A^+} \) represents the TIC signal. If it is assumed, as before, that all thermal ions are collected with the same efficiency, then equation (50) can be written

\[
i_{\text{TOT}} = i_{A^+} (i_{T_2^+} + i_{R_T^2}) / i_A^+ + \beta^{-1} i_{T_2^+}
\]

or

\[
\beta = \frac{i_{A^+} i_{\text{TOT}}}{i_A^+ i_{\text{TOT}} - i_{A^+} (i_{T_2^+} + i_{R_T^2})}
\]

(52)
Equation (52) gives the desired expression for $\beta$, in terms of measurable quantities.

Another difficulty arises when considering the collection efficiencies associated with electron-atom collisions. In this instance multiple ionization is possible for a 1000 ev electron beam. For the reactions

$$e + T_2 \rightarrow e + T^+_2 + e'$$
$$e + T + T + e'$$
$$e + T^{++}_2 + 2e'$$

(and higher multiple ionizations)

the following equation may be written:

$$i_{TOT} = \kappa^{-1} (i_{T^{+}_2} + i_{T^{++}_2} + \ldots) + \beta^{-1} i_{T^+_2} \quad (53)$$

where all molecular ions are again assumed to have the same collection efficiency $\kappa$. A second equation involving $\kappa$, similar to equation (51), can be obtained only if the probability for multiple ionization is known relative to single ionization. Massey and Burhop (1969) have tabulated multiple ionization cross sections for 1000 ev electrons incident upon several species. Their table shows that for argon the probability of double ionization is approximately 4.8% of the probability for single ionization, and the probability for multiple ionization greater than two is negligible. Therefore the expression
for $\alpha$ may be written

$$\alpha = \frac{i_A'}{.95 i_{TIC}}$$

where $i_{TIC}$ is the TIC signal. Combining this expression with equation (53) gives $\beta$. 
CHAPTER VI

Conclusion

A crossed-beam vacuum system which will be used for chemi-ionization measurements has been designed and constructed, and an interaction region pressure of $5 \times 10^{-9}$ torr can be consistently maintained for extended periods of time.

Most of the internal apparatus has been installed. The multichannel arrays have been properly aligned along the beam axes, and the target beam array half-widths and centerline intensities for various driving pressures have been examined. The total ion collection system, which includes the total ion collector (TIC), counting system, calibration electron gun, and faraday cup, is functioning properly. The mass spectrometer system has been designed and is presently being constructed.

The first experimental studies will involve collisions between helium atoms residing in metastable states and several stable neutral species of aeronomic interest, including $\text{H}_2$, $\text{N}_2$, and $\text{O}_2$. Studies will also be conducted on $\text{He}^*-\text{H}$ and $\text{He}^*-\text{O}$ collisions. These studies will include the determination of ionization cross sections, mass spectrometer analysis of product ions, energy analysis of the Penning electrons, and dependence of ionization cross sections upon relative velocities between colliding particles.
APPENDIX

A technique that is particularly useful for predicting the behavior of an ionized beam of particles in electric or magnetic fields involves the matrix formulation of beam trajectories. In the following sections the trajectory equations for a drift space, an electrostatic quadrupole lens, and a sector magnet are developed. Image width calculations for an ion beam at the focal point of a sector magnet are presented in Section B.

(A) Trajectory Equations

(1) Drift Space

A drift space is defined as any field free region of space. Consider the figure below, where the drift space is the region between the two dotted lines separated by distance L.

\[ \begin{align*}
\chi & \quad \chi_f \\
\xi & \quad L \quad \xi_f \\
\end{align*} \]

Assuming that a particle initially starts at point \((z_o, x_o)\) with slope \(\frac{dx}{dz} = x'_o\), we wish to predict the exit coordinates and slope after the particle has traversed the drift space. At \(z = z_f\) we find, by using the equation for a straight line,
The exit slope is \( x'_f = x'_o \), since in the absence of any external fields the particle experiences no deflecting forces, thereby retaining its initial slope. Equation (A1) and the expression for \( x'_f \) can be combined into the following matrix equation:

\[
\begin{pmatrix}
  x \\
  x' \\
\end{pmatrix}_f =
\begin{pmatrix}
  1 & L \\
  0 & 1 \\
\end{pmatrix}
\begin{pmatrix}
  x \\
  x' \\
\end{pmatrix}_o
\]

\[
= M_{DS}
\begin{pmatrix}
  x \\
  x' \\
\end{pmatrix}_o
\]

where

\[
M_{DS} =
\begin{pmatrix}
  1 & L \\
  0 & 1 \\
\end{pmatrix}
\]

is the matrix representing a drift space of length \( L \). We see from equation (A2) that if initial conditions \( x_o \) and \( x'_o \) are known and \( L \) is known then the final conditions are easily calculable.

(2) Quadrupole Lens

In a quadrupole lens charged particles are subject to
a field described by a potential distribution of the form (Livingston and Blewett, 1962)

\[ V = \text{constant} \ (x^2 - y^2) \]  \hspace{1cm} (A3)

where the x and y-axes are indicated in Figure (A1). The equipotentials for this field configuration are rectangular hyperbolas. In practice, this situation is usually approximated by using cylinders with circular cross-sectional areas instead of ones having hyperbolic cross-sectional areas, thereby making construction of the quadrupole lens electrodes much easier. The two cylinders whose centers lie on the x-axis have potentials \( +V_0 \), while the two remaining cylinders have potentials \( -V_0 \). A beam of charged particles is assumed to enter the quadrupole lens at \( z = 0 \) with initial coordinates \((x,y,0)\).

If the particles are ions, it is evident from the signs of the electrode potentials that the particles will experience a converging (focusing) force in the x-direction and a diverging (defocusing) force in the y-direction.

Consider the equations of motion for the x-z and y-z planes:

\[ m\ddot{x} = eE_x \]

\[ m\ddot{y} = eE_y \]

Since \( \mathbf{E} = -\nabla V \) these equations become, with the help of equation (A3),
Figure A1

Quadrupole Lens
\[ mx'' = -ex \cdot \text{constant} \]
\[ my' = +ey \cdot \text{constant} \]

If these differential equations are solved subject to the initial conditions on position \((x'_0, y'_0, 0)\) and direction \((x'_0, y'_0)\) at \(z=0\), we find

\[ x = x'_0 \cos(kz) + \frac{x'_0}{k} \sin(kz) \] \hspace{1cm} (A4)
\[ y = y'_0 \cosh(kz) + \frac{y'_0}{k} \sinh(kz) \] \hspace{1cm} (A5)

where \[ k = a^{-1} \left( \frac{V}{V_{\text{ion}}} \right)^{1/2}. \] \hspace{1cm} (A6)

\(V_{\text{ion}}\) is the potential associated with the kinetic energy of the ion at the entrance to the quadrupole lens, and \(a\) is defined in Figure (A1).

Differentiating these equations with respect to \(z\) gives

\[ x' = -kx'_0 \sin(kz) + x'_0 \cos(kz) \] \hspace{1cm} (A7)
\[ y' = ky'_0 \sinh(kz) + y'_0 \cosh(kz) \] \hspace{1cm} (A8)

Combining equations (A4) through (A8) leads to the following matrix equations. For the \(x-z\) plane,

\[
\begin{pmatrix}
  x \\
  x' \\
  z
\end{pmatrix} =
\begin{pmatrix}
  \cos(kz) & k^{-1} \sin(kz) \\
  -k \sin(kz) & \cos(kz)
\end{pmatrix}
\begin{pmatrix}
  x \\
  x'
\end{pmatrix}
\] \hspace{1cm} (A9)
where \( M_{\text{con}} \), the matrix representing the converging plane, is
\[
M_{\text{con}} = \begin{pmatrix}
\cos(kz) & k^{-1}\sin(kz) \\
-k \sin(kz) & \cos(kz)
\end{pmatrix}
\]

For the \( y-z \) plane,
\[
\begin{pmatrix}
y \\
y'
\end{pmatrix}
= \begin{pmatrix}
\cosh(kz) & k^{-1}\sinh(kz) \\
k \sinh(kz) & \cosh(kz)
\end{pmatrix}
\begin{pmatrix}
y \\
y'
\end{pmatrix}
\]
\( (A10) \)

where \( M_{\text{div}} \), the matrix for the diverging plane, is
\[
M_{\text{div}} = \begin{pmatrix}
\cosh(kz) & k^{-1}\sinh(kz) \\
k \sinh(kz) & \cosh(kz)
\end{pmatrix}
\]

(3) Sector Magnet

The geometry of a sector magnet is shown in Figure (A2). The reference particle trajectory, known as the median ray, is characterized by radial plane coordinates \( x=0 \) and \( \theta=0 \) everywhere and has momentum \( P \). It is assumed that the median ray enters and exits the magnet at right angles to the magnet edges, and that it lies on radius \( r \) while inside the magnet. An arbitrary ray of Figure (A2) has initial distance \( x_0 \) and slope \( \theta_0 \) and enters the magnet with momentum \( P' = P + \Delta P \).

In order to relate \( r \) and \( P \), we equate the centrifugal force with the magnetic part of the Lorentz force for an
Figure A2

Sector magnet geometry for calculations of section A-3 in Appendix.
ion inside the magnet:

\[ \frac{mv^2}{r} = evB \]

where \( e \) is the charge on the ion of mass \( m \) and velocity \( v \), and \( B \) is the magnetic field strength, assumed to be a constant inside the magnet. Solving for the momentum of the ion,

\[ P = mv = eBr \] (A11)

Also,

\[ \frac{dP}{dr} = eB \] (A12)

Combining equations (A11) and (A12),

\[ \frac{P}{r} = \frac{dP}{dr} \]

or

\[ \frac{dP}{P} = \frac{dr}{r} \] (A13)

We now wish to derive a matrix equation relating exit distance \( x \) and slope \( \theta \) to the entrance distance \( x_o \) and slope \( \theta_o \), using the forgoing information. The derivation which follows is based upon a paper by S. Penner (1961).

Figure (A2) gives two expressions for OD:

\[ OD = OC + CD \]

\[ OD = OR + RD \]
Equating these two equations gives

\[ CD = x = RD - OC + OR. \]

But

\[ RD = PD \cos \theta \]
\[ = r' \cos \theta \]
\[ = (r + \Delta r) \cos \theta, \]

where \( r = r' - r \), and

\[ OC = r, \]

giving

\[ x = (r + \Delta r) \cdot \cos \theta - r + OR. \quad \text{(A14)} \]

If we now consider an enlargement of the bottom portion of Figure (A2), shown below, and construct parallelogram QPGF,

we obtain

\[ OR = OF + FR \]
\[ = OQ \sin \alpha + FG \cos \alpha \]
\[ = OQ \sin \alpha + PQ \cos \alpha. \]
Using this expression in equation (A14), we find

\[ x = (r + \Delta r)\cos\theta - r + OQ \sin\alpha + PQ \cos\alpha. \quad (A15) \]

To obtain expressions for OQ and PQ, we consider another portion of Figure (A2), shown in the diagram below.

We see that

\[ OQ = HP = (r + \Delta r)\sin\theta_o. \quad (A16) \]

Also,

\[ OB = OH + HB = PQ + PB \cdot \cos\theta_o = PQ + (r + \Delta r)\cos\theta_o \]

or

\[ PQ = OB - (r + \Delta r) \cos\theta_o. \]

But, from the above figure,

\[ OB = OA + AB = r + x_o, \]

giving

\[ PQ = r + x_o - (r + \Delta r) \cos\theta_o. \quad (A17) \]

Using equations (A16) and (A17) in (A15) gives

\[ x = (r + \Delta r)\cos\theta - r + (r + \Delta r)\sin\theta_o + \cos\alpha \left[ r + x_o - (r + \Delta r) \cos\theta_o \right]. \quad (A18) \]
which is an exact expression.

In many cases of interest the following assumptions can be made:

\[ \theta \text{ and } \theta_0 \ll 1 \]
\[ \Delta r \text{ and } x_0 \ll r . \]

Equation (A18) then reduces to

\[ x = r_0 \cdot \sin \alpha + x_0 \cdot \cos \alpha + \Delta r (1 - \cos \alpha) \quad \text{(A19)} \]

which is an expression for the exit distance in terms of initial conditions, \( r \), and \( \alpha \), as desired.

To get a corresponding expression for \( \theta \) we note that \( \tan \theta \) represents the slope of the exit ray, i.e. the change in \( x \) divided by the arc length traversed:

\[ \tan \theta = \frac{\Delta x}{\Delta S} \quad \frac{\Delta \alpha}{\Delta S} . \quad \text{(A20)} \]

But \( S = \alpha r \) so that \[ \frac{\Delta \alpha}{\Delta S} = \frac{1}{r} \]
giving, by equation (A20),

\[ \tan \theta = r^{-1} \frac{dx}{d\alpha} . \quad \text{(A21)} \]

From equation (A19),
\[ \frac{dx}{d\alpha} = r_0 \cdot \cos \kappa - x_0 \cdot \sin \kappa + \Delta r \sin \kappa \]

so that for small \( \theta \) equation (A21) becomes

\[ \theta = \theta_0 \cos \kappa - x_0 \sin \kappa/r + \Delta r \sin \kappa/r . \quad (A22) \]

In order that a matrix equation can be written, we choose to eliminate \( \Delta r \) from equations (A19) and (A22) with the aid of equation (A13). The results are

\[ x = r_0 \cdot \sin \kappa + x_0 \cdot \cos \kappa + r \Delta P (1 - \cos \kappa) / \rho \]

\[ \theta = \theta_0 \cos \kappa - x_0 \cdot \sin \kappa/r + \Delta P \cdot \sin \kappa / \rho . \]

If we also include a third equation,

\[ \Delta P/\rho = \Delta P/\rho \]

we finally obtain the desired matrix equation:

\[
\begin{pmatrix}
  x \\
  \theta \\
  \Delta P/\rho
\end{pmatrix}
= \begin{pmatrix}
  \cos \kappa & r \cdot \sin \kappa & r (1 - \cos \kappa) \\
  -r^{-1} \sin \kappa & \cos \kappa & \sin \kappa \\
  0 & 0 & 1
\end{pmatrix}
\begin{pmatrix}
  x \\
  \theta \\
  \Delta P/\rho
\end{pmatrix}
\]

\[ = M_{\text{sector}} \begin{pmatrix}
  x \\
  \theta \\
  \Delta P/\rho
\end{pmatrix}, \quad (A23) \]
When calculating trajectories in systems containing both sector magnets and quadrupole lenses (or drift spaces), we can easily change $M_{\text{con}}$ and $M_{\text{div}}$ (or $M_{DS}$) into 3x3 matrices by inspection. For example,

$$M_{\text{con}}^{3x3} = \begin{pmatrix} M_{\text{con}}^{2x2} & 0 \\ - & - \\ 0 & 0 & 1 \end{pmatrix}$$

(A24)

The net effect of a combination of sector magnets, quadrupole lenses, and drift spaces is then represented by the product of the appropriate transfer matrices. For the case discussed in Chapter V, which is composed of the elements shown in the block diagram below,

\[
\begin{array}{c}
\text{entrance} \rightarrow \text{QL1} \rightarrow \text{DS1} \rightarrow \text{QL2} \rightarrow \text{DS2} \rightarrow \text{Sector} \rightarrow \text{DS3} \rightarrow \text{exit}
\end{array}
\]

we may write

$$\begin{pmatrix} x \\ x' \end{pmatrix} = M_{DS3} M_{\text{Sector}} M_{DS2} M_{QL2} M_{DS1} M_{QL1} \begin{pmatrix} x \\ x' \end{pmatrix}_{\text{final}}$$

where $\theta = x'$. 
(B) Image Width

The image width of a sector magnet is defined as the transverse dimension of the ion beam, perpendicular to the median ray, at the focal point. We wish to calculate the image width for a sector magnet which is being operated in the parallel beam mode of Chapter V, where all ion trajectories at the magnet entrance are parallel to the median ray (see figure below).

Figure A3

The median ray enters the magnetic field at A, moves along radius \( r = OA \), exits at C and passes through \( F' \). Another ray follows radius \( r' = PB \) through the magnet, exits at an angle \( \theta \) with respect to the field boundary, and passes through \( F \).

From the figure, we find two expressions for \( OP \):

\[
OP = \frac{PR}{\sin \alpha}
\]

\[
OP + PB = OA + AB
\]
Eliminating OP from these two equations gives

\[ PR = (OA + AB - PB) \sin \alpha \]
\[ = (r + x_o - r') \sin \alpha \]  \hspace{1cm} (A25)

Also,
\[ \sin \theta = \frac{PR}{PD} \]

or, using equation (A25),

\[ \sin \theta = \frac{(r - r' + x_o) \cdot \sin \alpha}{PD} \]
\[ = \frac{(x_o - \Delta r) \cdot \sin \alpha}{r'} \]  \hspace{1cm} (A26)

where
\[ \Delta r = r' - r. \]

Again referring to the figure, we obtain

\[ OC + CD = OR + RD \]

or
\[ x = CD = OR + RD - OC \]
\[ = OR + RD - r. \]  \hspace{1cm} (A27)

But
\[ OR = OP \cdot \cos \alpha \]
\[ = (x_o - \Delta r) \cdot \cos \alpha \]  \hspace{1cm} (A28)

and
\[ RD = PD \cos \theta \]
\[ = r' \cdot \cos \theta. \]  \hspace{1cm} (A29)
Using equations (A28) and (A29) in (A27),

\[ x = (x_0 - \Delta x) \cdot \cos \alpha + r' \cdot \cos \theta - r. \]

To eliminate \( \theta \), we note that \( \cos \theta = (1 - \sin^2 \theta)^{1/2} \) and use equation (A26) for \( \sin \theta \):

\[ x = (x_0 - \Delta x) \cdot \cos \alpha + r' \left[ 1 - \frac{(x_0 - \Delta x)^2}{r'^2 \sin^2 \alpha} \right]^{1/2} - r. \]  

(A30)

If vertical line DE is constructed in the preceding figure, we find, for the arbitrary ray,

\[ OF = OE + EF \]
\[ = OD \sin (\angle ODE) + DE \tan (\angle DFE) \]
\[ = (r + x) \sin \alpha + \left[ (r + x) \cos \alpha \right] \tan (\alpha + \theta). \]  

(A31)

If vertical line CE' in constructed, we find, for the median ray,

\[ OF' = OE' + E'F' \]
\[ = r \cdot \sin \alpha + (r \cdot \cos \alpha) \cdot \tan \alpha. \]  

(A32)

Subtraction of equation (A32) from (A31) gives
\[
OF' - OF = x \cdot \sin \kappa + (r+x) \cdot \cos \kappa \cdot \text{ctn} (\kappa + \theta) - r \cdot \cos \kappa \cdot \text{ctn} \kappa
\]

\[
= x \left[ \sin \kappa + \cos \kappa \cdot \text{ctn} (\kappa + \theta) \right] + r \cdot \cos \kappa \left[ \text{ctn} (\kappa + \theta) - \text{ctn} \kappa \right]
\]

This equation does not correspond to the image width, since \(OF - OF'\) is not measured perpendicular to the median ray. However, the image width \(W\) is easily found by noting that

\[
W = (OF - OF') \cdot \sin \kappa,
\]

which leads to the desired expression

\[
W = \left\{ x \left[ \sin \kappa + \cos \kappa \cdot \text{ctn} (\kappa + \theta) \right] + r \cdot \cos \kappa \left[ \text{ctn} (\kappa + \theta) - \text{ctn} \kappa \right] \right\} \sin \kappa,
\]

(A33)
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